Full wwPDB EM Validation Report

Nov 29, 2022 – 02:12 AM JST

PDB ID	:	7VNY
EMDB ID	:	EMD-32047
Title	:	Rba sphaeroides WT RC-LH1 monomer
Authors	:	Bracun, L.; Yamagata, A.; Liu, L.N.; Shirouzu, M.
Deposited on	:	2021-10-12
Resolution	:	2.79 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

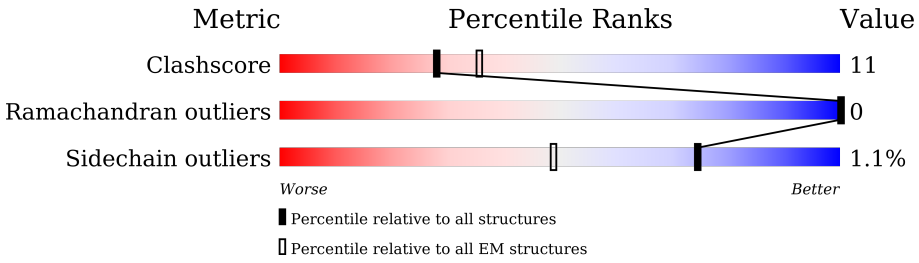
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	282	83% 17%
2	M	308	81% 18%
3	H	260	7% 79% 15% 5%
4	1	58	38% 74% 17% 9%
4	3	58	17% 74% 19% 7%
4	7	58	10% 62% 17% 21%
4	9	58	5% 78% 16% 7%
4	A	58	69% 24% 7%

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Mol	Chain	Length	Quality of chain
4	D	58	7% 79% 14% 7%
4	F	58	7% 78% 16% 7%
4	I	58	84% 9% 7%
4	K	58	9% 69% 24% 7%
4	O	58	7% 71% 21% 7%
4	Q	58	9% 76% 17% 7%
4	S	58	5% 83% 9% 7%
4	U	58	7% 83% 10% 7%
4	W	58	12% 72% 21% 7%
5	0	49	6% 78% 12% 10%
5	2	49	41% 67% 12% 20%
5	8	49	10% 73% 16% 10%
5	B	49	6% 67% 24% 8%
5	C	49	22% 67% 20% 12%
5	E	49	6% 61% 27% 12%
5	G	49	10% 71% 16% 12%
5	J	49	12% 69% 18% 12%
5	N	49	14% 69% 18% 12%
5	P	49	14% 82% 6% 12%
5	R	49	14% 63% 24% 12%
5	T	49	14% 73% 14% 12%
5	V	49	16% 73% 14% 12%
5	Z	49	29% 76% 10% 14%
6	X	82	44% 41% 22% 37%
7	Y	53	21% 77% 17% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	SPO	0	101	-	X	-	-
13	SPO	3	102	-	X	-	-
13	SPO	3	104	-	X	-	-
13	SPO	8	102	-	X	-	-
13	SPO	9	102	-	X	-	-
13	SPO	B	101	-	X	-	-
13	SPO	D	102	-	X	-	-
13	SPO	D	103	-	X	-	-
13	SPO	E	102	-	X	-	-
13	SPO	F	102	-	X	-	-
13	SPO	G	101	-	X	-	-
13	SPO	I	102	-	X	-	-
13	SPO	J	101	-	X	-	-
13	SPO	J	103	-	X	-	-
13	SPO	M	405	-	X	-	-
13	SPO	N	102	-	X	-	-
13	SPO	O	102	-	X	-	-
13	SPO	O	104	-	X	-	-
13	SPO	P	101	-	X	-	-
13	SPO	T	101	-	X	-	-
13	SPO	T	102	-	X	-	-
13	SPO	U	102	-	X	-	-
13	SPO	U	104	-	X	-	-
13	SPO	V	101	-	X	-	-
13	SPO	W	103	-	X	-	-
13	SPO	X	101	-	X	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 22472 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	281	2232	1507	355	362	8	0	0

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	305	2431	1623	397	400	11	0	0

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	247	1875	1202	318	345	10	0	0

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	54	455	310	73	69	3	0	0
4	D	54	455	310	73	69	3	0	0
4	F	54	455	310	73	69	3	0	0
4	I	54	455	310	73	69	3	0	0
4	K	54	455	310	73	69	3	0	0
4	O	54	455	310	73	69	3	0	0
4	Q	54	455	310	73	69	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	U	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	W	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	3	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	1	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	7	46	Total	C	N	O	S	0	0
			392	271	60	58	3		
4	9	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

- Molecule 5 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
5	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	G	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	N	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	P	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	R	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	T	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	V	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	C	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	Z	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
5	2	39	Total	C	N	O	S	0	0
			316	210	51	54	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	0	44	Total	C	N	O	S	0	0
			359	240	56	62	1		

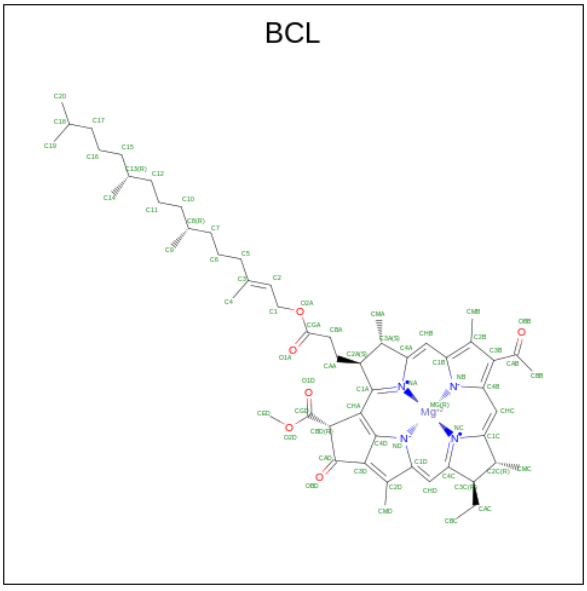
- Molecule 6 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	52	Total	C	N	O	S	0	0
			406	270	71	62	3		

- Molecule 7 is a protein called Rsp_7571 Protein-Y PufY.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	50	Total	C	N	O	S	0	0
			368	250	57	58	3		

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	L	1	Total	C	Mg	N	O	0
			195	162	3	12	18	
8	L	1	Total	C	Mg	N	O	0
			195	162	3	12	18	

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Mol	Chain	Residues	Atoms					AltConf
8	L	1	Total	C	Mg	N	O	0
			195	162	3	12	18	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	A	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	F	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	F	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	O	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	O	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	S	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	S	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	U	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	U	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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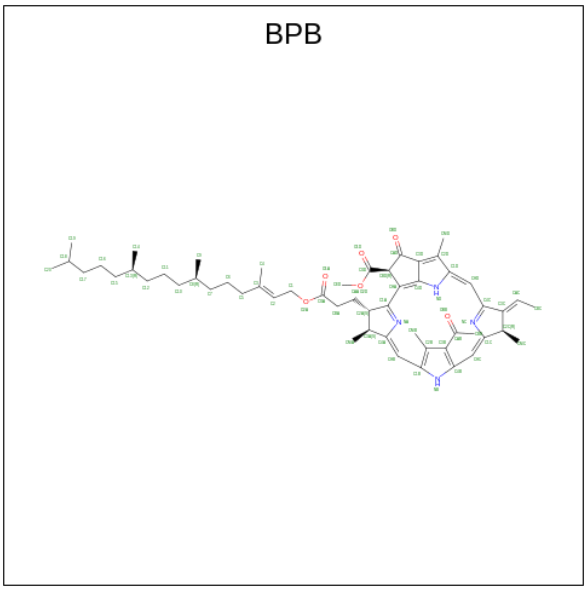
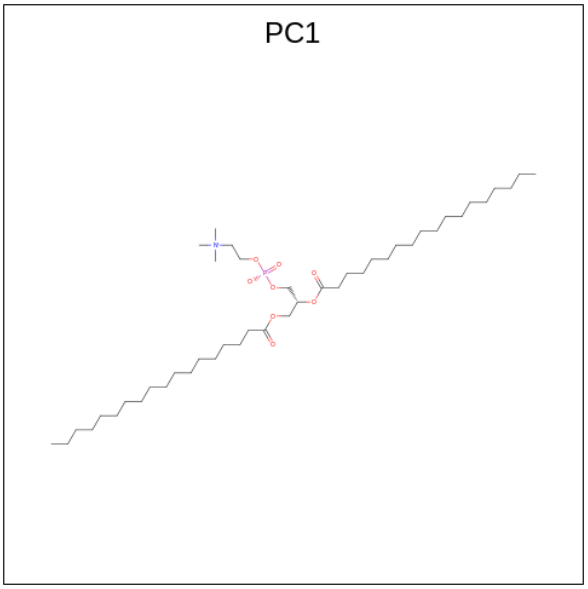
Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	3	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	3	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	1	1	Total	C	Mg	N	O	0
			117	95	2	8	12	
8	1	1	Total	C	Mg	N	O	0
			117	95	2	8	12	
8	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	8	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



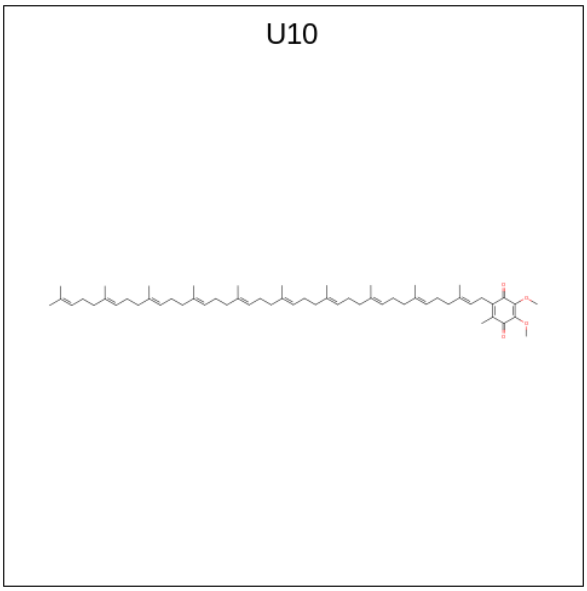
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			62	52	4	6	
9	M	1	Total	C	N	O	0
			55	45	4	6	

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	L	1	Total	C	N	O	P	0
			71	51	2	16	2	
10	L	1	Total	C	N	O	P	0
			71	51	2	16	2	
10	H	1	Total	C	N	O	P	0
			102	72	3	24	3	
10	H	1	Total	C	N	O	P	0
			102	72	3	24	3	
10	H	1	Total	C	N	O	P	0
			102	72	3	24	3	
10	A	1	Total	C	N	O	P	0
			77	57	2	16	2	
10	A	1	Total	C	N	O	P	0
			77	57	2	16	2	
10	D	1	Total	C	N	O	P	0
			37	27	1	8	1	
10	W	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

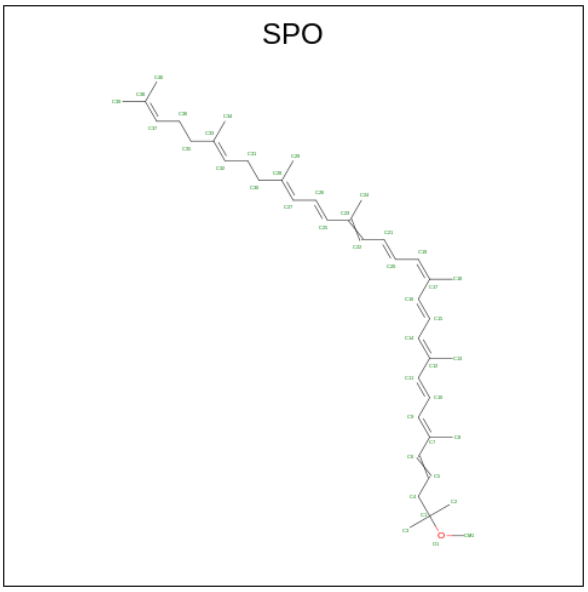


Mol	Chain	Residues	Atoms	AltConf
11	L	1	Total C O 81 73 8	0
11	L	1	Total C O 81 73 8	0
11	M	1	Total C O 48 44 4	0
11	Y	1	Total C O 38 34 4	0

- Molecule 12 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
12	M	1	Total Fe 1 1	0

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
13	M	1	Total C O 42 41 1	0
13	B	1	Total C O 42 41 1	0
13	D	1	Total C O 84 82 2	0
13	D	1	Total C O 84 82 2	0
13	E	1	Total C O 42 41 1	0
13	F	1	Total C O 42 41 1	0
13	G	1	Total C O 42 41 1	0
13	I	1	Total C O 42 41 1	0
13	J	1	Total C O 84 82 2	0
13	J	1	Total C O 84 82 2	0
13	N	1	Total C O 42 41 1	0
13	O	1	Total C O 84 82 2	0
13	O	1	Total C O 84 82 2	0
13	P	1	Total C O 42 41 1	0

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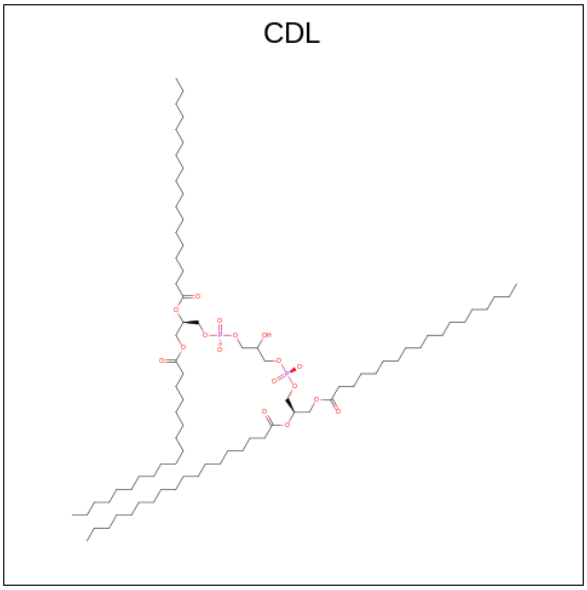
Mol	Chain	Residues	Atoms	AltConf
13	T	1	Total C O 84 82 2	0
13	T	1	Total C O 84 82 2	0
13	U	1	Total C O 84 82 2	0
13	U	1	Total C O 84 82 2	0
13	V	1	Total C O 42 41 1	0
13	W	1	Total C O 42 41 1	0
13	3	1	Total C O 84 82 2	0
13	3	1	Total C O 84 82 2	0
13	8	1	Total C O 42 41 1	0
13	9	1	Total C O 42 41 1	0
13	0	1	Total C O 42 41 1	0
13	X	1	Total C O 39 38 1	0

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



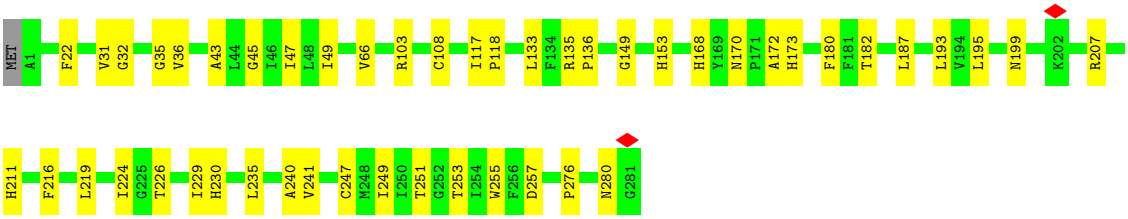
Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	O	P	0
			100	81	17	2	
14	H	1	Total	C	O	P	0
			78	59	17	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

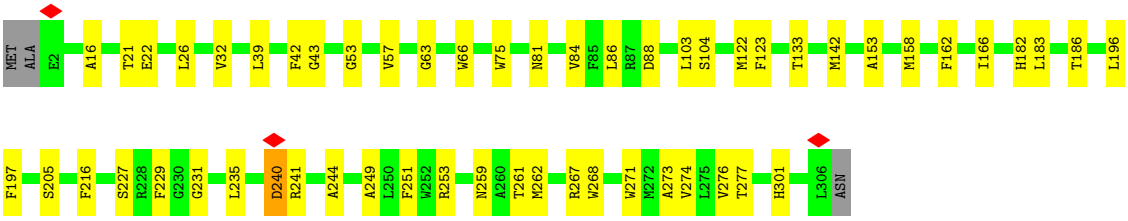
• Molecule 1: Reaction center protein L chain

Chain L:



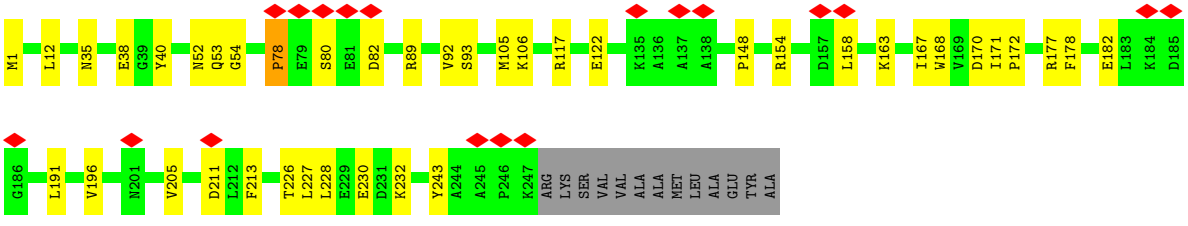
• Molecule 2: Reaction center protein M chain

Chain M:



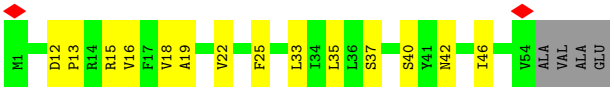
• Molecule 3: Reaction center protein H chain

Chain H:



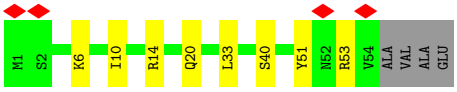
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain A:



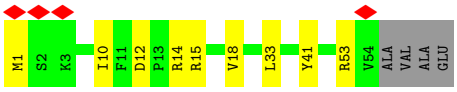
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain D:



• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain F:

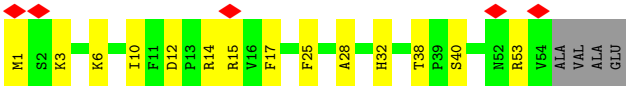


• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain I:

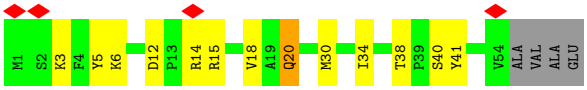
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain K:



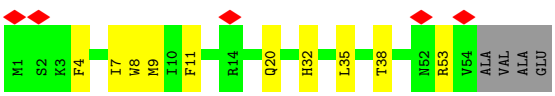
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain O:



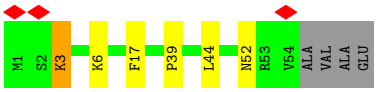
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain Q:



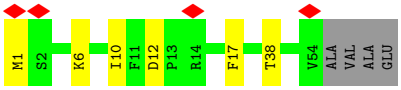
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain S:



• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain U:

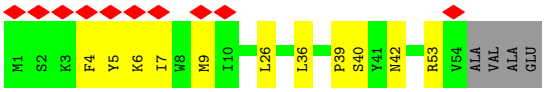


• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain W:

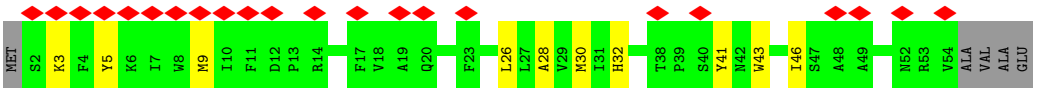
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 3:



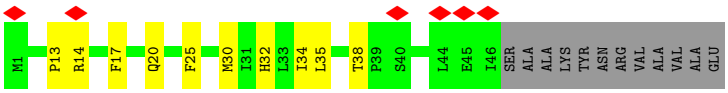
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 1:



• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 7:

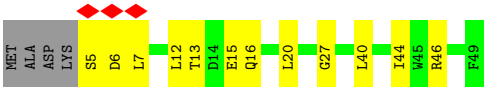


• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 9:

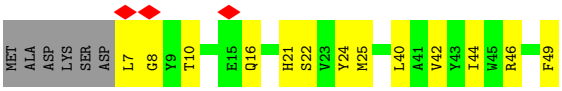
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain B:



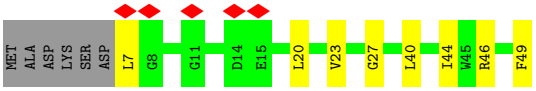
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain E:



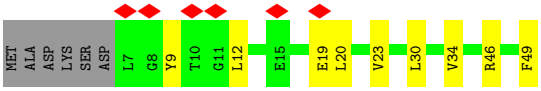
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain G:



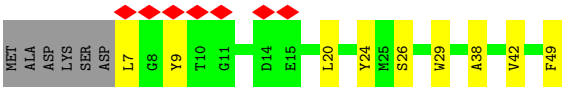
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain J:



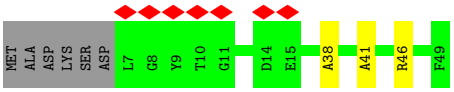
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain N:



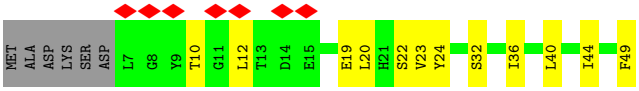
• Molecule 5: Light-harvesting protein B-875 beta chain

Chain P:

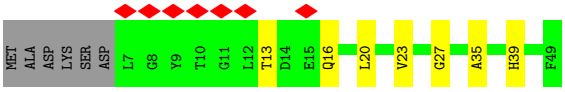


• Molecule 5: Light-harvesting protein B-875 beta chain

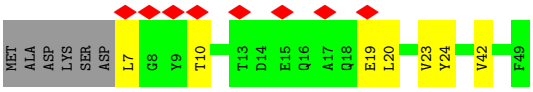
Chain R:



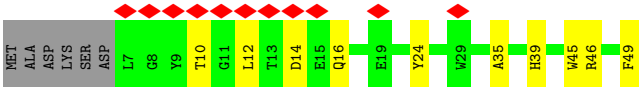
• Molecule 5: Light-harvesting protein B-875 beta chain



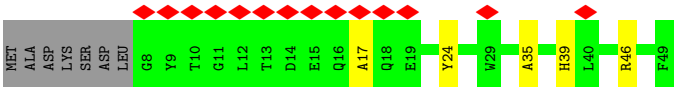
• Molecule 5: Light-harvesting protein B-875 beta chain



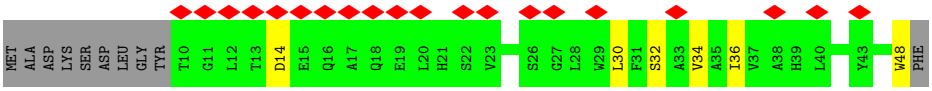
• Molecule 5: Light-harvesting protein B-875 beta chain



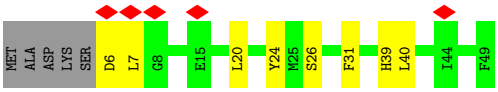
• Molecule 5: Light-harvesting protein B-875 beta chain



• Molecule 5: Light-harvesting protein B-875 beta chain

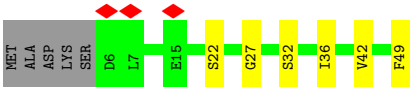


• Molecule 5: Light-harvesting protein B-875 beta chain



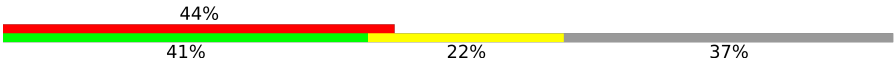
• Molecule 5: Light-harvesting protein B-875 beta chain

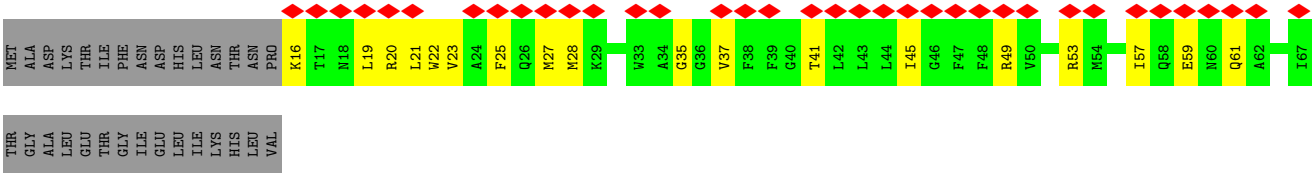
Chain 0:



• Molecule 6: Intrinsic membrane protein PufX

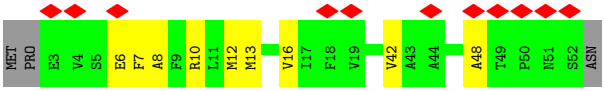
Chain X:





• Molecule 7: Rsp_7571 Protein-Y PufY

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68554	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45.026	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.295	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	265.0, 265.0, 265.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BPB, SPO, U10, FE2, CDL, BCL, PC1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	L	0.31	0/2320	0.48	0/3175
2	M	0.32	0/2524	0.50	0/3446
3	H	0.31	0/1925	0.58	2/2620 (0.1%)
4	1	0.27	0/461	0.45	0/625
4	3	0.29	0/469	0.49	0/635
4	7	0.29	0/405	0.45	0/549
4	9	0.31	0/469	0.46	0/635
4	A	0.29	0/469	0.45	0/635
4	D	0.30	0/469	0.46	0/635
4	F	0.33	0/469	0.48	0/635
4	I	0.30	0/469	0.45	0/635
4	K	0.32	0/469	0.51	0/635
4	O	0.31	0/469	0.48	0/635
4	Q	0.33	0/469	0.50	0/635
4	S	0.34	0/469	0.54	1/635 (0.2%)
4	U	0.32	0/469	0.46	0/635
4	W	0.33	0/469	0.52	0/635
5	0	0.31	0/372	0.46	0/510
5	2	0.31	0/327	0.50	0/449
5	8	0.30	0/372	0.48	0/510
5	B	0.31	0/378	0.48	0/518
5	C	0.28	0/364	0.42	0/499
5	E	0.31	0/364	0.46	0/499
5	G	0.29	0/364	0.45	0/499
5	J	0.31	0/364	0.49	0/499
5	N	0.30	0/364	0.45	0/499
5	P	0.29	0/364	0.44	0/499
5	R	0.30	0/364	0.44	0/499
5	T	0.29	0/364	0.45	0/499
5	V	0.29	0/364	0.50	0/499
5	Z	0.27	0/356	0.46	0/488
6	X	0.28	0/417	0.51	0/563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
7	Y	0.29	0/379	0.45	0/513
All	All	0.31	0/19140	0.49	3/26077 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	78	PRO	CA-N-CD	-11.54	95.34	111.50
3	H	78	PRO	N-CD-CG	-5.86	94.41	103.20
4	S	39	PRO	CA-N-CD	-5.16	104.27	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	37	0
2	M	2431	0	2345	46	0
3	H	1875	0	1877	31	0
4	1	447	0	465	6	0
4	3	455	0	477	7	0
4	7	392	0	412	11	0
4	9	455	0	477	7	0
4	A	455	0	477	12	0
4	D	455	0	477	7	0
4	F	455	0	477	8	0
4	I	455	0	477	5	0
4	K	455	0	477	9	0
4	O	455	0	477	9	0
4	Q	455	0	477	8	0
4	S	455	0	477	6	0
4	U	455	0	477	6	0
4	W	455	0	477	13	0
5	0	359	0	340	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	2	316	0	304	4	0
5	8	359	0	340	10	0
5	B	365	0	345	9	0
5	C	351	0	336	10	0
5	E	351	0	336	13	0
5	G	351	0	336	7	0
5	J	351	0	336	7	0
5	N	351	0	336	12	0
5	P	351	0	336	4	0
5	R	351	0	336	9	0
5	T	351	0	336	5	0
5	V	351	0	336	7	0
5	Z	343	0	325	4	0
6	X	406	0	420	17	0
7	Y	368	0	363	6	0
8	0	61	0	61	4	0
8	1	117	0	112	3	0
8	3	132	0	148	2	0
8	7	66	0	74	10	0
8	8	61	0	61	4	0
8	9	66	0	74	3	0
8	A	132	0	148	10	0
8	C	66	0	74	2	0
8	D	66	0	74	2	0
8	E	66	0	74	2	0
8	F	132	0	148	6	0
8	I	66	0	74	1	0
8	J	66	0	74	6	0
8	K	66	0	74	0	0
8	L	195	0	213	7	0
8	M	66	0	74	2	0
8	N	66	0	74	5	0
8	O	132	0	148	4	0
8	Q	66	0	74	2	0
8	R	66	0	74	7	0
8	S	132	0	148	8	0
8	U	132	0	148	10	0
8	W	66	0	74	4	0
9	L	62	0	65	4	0
9	M	55	0	51	5	0
10	A	77	0	105	13	0
10	D	37	0	48	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	102	0	130	11	0
10	L	71	0	90	3	0
10	W	37	0	48	5	0
11	L	81	0	102	6	0
11	M	48	0	63	3	0
11	Y	38	0	47	2	0
12	M	1	0	0	0	0
13	0	42	0	59	8	0
13	3	84	0	117	16	0
13	8	42	0	59	5	0
13	9	42	0	60	5	0
13	B	42	0	60	10	0
13	D	84	0	119	12	0
13	E	42	0	60	4	0
13	F	42	0	59	8	0
13	G	42	0	58	6	0
13	I	42	0	59	7	0
13	J	84	0	117	11	0
13	M	42	0	60	7	0
13	N	42	0	60	8	0
13	O	84	0	120	11	0
13	P	42	0	58	5	0
13	T	84	0	120	16	0
13	U	84	0	119	12	0
13	V	42	0	59	8	0
13	W	42	0	60	7	0
13	X	39	0	53	6	0
14	H	78	0	106	6	0
14	M	100	0	156	4	0
All	All	22472	0	23315	483	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (483) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:7:LEU:HD23	5:C:16:GLN:HE22	1.44	0.82
4:S:6:LYS:NZ	5:V:19:GLU:OE2	2.13	0.81
4:3:40:SER:O	5:Z:46:ARG:NH1	2.15	0.80
2:M:153:ALA:HA	2:M:277:THR:HG21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:102:SPO:H131	13:N:102:SPO:H16	1.64	0.78
4:D:6:LYS:HB3	13:F:102:SPO:H402	1.66	0.77
8:U:103:BCL:H203	13:V:101:SPO:H11	1.65	0.76
13:U:102:SPO:H15	8:W:102:BCL:H92	1.67	0.76
4:O:38:THR:OG1	4:O:40:SER:O	2.04	0.75
4:D:10:ILE:HG23	4:F:14:ARG:HG2	1.68	0.74
1:L:187:LEU:HD13	2:M:216:PHE:HB2	1.69	0.73
13:0:101:SPO:H131	13:0:101:SPO:H183	1.70	0.72
4:D:40:SER:O	5:E:46:ARG:NH1	2.23	0.72
4:S:3:LYS:HG3	4:S:6:LYS:HD2	1.71	0.71
5:B:20:LEU:HG	13:B:101:SPO:H352	1.71	0.70
2:M:301:HIS:HD2	10:H:301:PC1:H11	1.56	0.70
13:8:102:SPO:H242	13:8:102:SPO:C27	2.23	0.69
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.75	0.69
5:J:49:PHE:CE2	13:J:103:SPO:H11	2.27	0.69
13:O:104:SPO:H352	5:R:20:LEU:HG	1.74	0.69
13:O:104:SPO:H26	13:P:101:SPO:H393	1.73	0.69
4:W:38:THR:OG1	4:W:40:SER:O	2.12	0.68
8:S:102:BCL:H2	8:S:102:BCL:H72	1.75	0.67
13:U:102:SPO:H361	5:V:23:VAL:HG11	1.76	0.67
4:W:6:LYS:HB3	13:3:102:SPO:H361	1.77	0.66
13:D:103:SPO:H182	13:D:103:SPO:H131	1.78	0.66
8:U:103:BCL:H72	8:U:103:BCL:H2	1.78	0.66
13:W:103:SPO:H301	5:C:24:TYR:HA	1.76	0.65
8:1:102:BCL:H71	8:1:102:BCL:HBB2	1.78	0.65
13:3:104:SPO:H14	13:3:104:SPO:H182	1.78	0.65
2:M:75:TRP:HE1	13:M:405:SPO:HM12	1.61	0.64
2:M:273:ALA:O	2:M:276:VAL:HG12	1.97	0.64
1:L:226:THR:O	1:L:230:HIS:ND1	2.24	0.64
11:M:404:U10:H212	10:H:302:PC1:H352	1.78	0.64
3:H:148:PRO:HD2	3:H:167:ILE:HD11	1.80	0.64
13:N:102:SPO:H132	5:P:41:ALA:HB1	1.80	0.64
13:E:102:SPO:H16	13:E:102:SPO:H131	1.78	0.64
8:A:103:BCL:H51	13:D:103:SPO:H243	1.80	0.64
10:H:301:PC1:H153	14:H:304:CDL:H511	1.80	0.64
2:M:268:TRP:HE1	3:H:35:ASN:ND2	1.96	0.63
3:H:80:SER:OG	3:H:82:ASP:OD1	2.12	0.63
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.79	0.63
1:L:247:CYS:O	1:L:251:THR:OG1	2.16	0.63
8:U:101:BCL:HHD	5:V:42:VAL:HG21	1.79	0.63
4:7:14:ARG:HG2	6:X:22:TRP:HZ2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:40:TYR:OH	10:H:302:PC1:O12	2.16	0.62
1:L:280:ASN:ND2	2:M:88:ASP:OD1	2.32	0.62
5:Z:35:ALA:O	5:Z:39:HIS:ND1	2.25	0.62
8:C:101:BCL:H52	13:3:104:SPO:H26	1.80	0.62
3:H:78:PRO:HD2	3:H:78:PRO:O	1.99	0.62
4:F:10:ILE:HD11	13:J:101:SPO:H393	1.82	0.62
4:D:20:GLN:OE1	5:E:24:TYR:OH	2.17	0.61
1:L:43:ALA:O	1:L:47:ILE:HD12	2.01	0.61
7:Y:8:ALA:O	7:Y:12:MET:HG3	2.00	0.61
2:M:253:ARG:HH22	10:H:302:PC1:H112	1.65	0.61
2:M:268:TRP:HE1	3:H:35:ASN:HD21	1.49	0.60
8:R:101:BCL:H51	13:T:102:SPO:H243	1.82	0.60
13:U:102:SPO:H302	5:V:24:TYR:HA	1.84	0.60
5:0:32:SER:O	5:0:36:ILE:HG13	2.01	0.60
4:A:18:VAL:HA	10:A:102:PC1:H292	1.83	0.59
4:S:6:LYS:HB2	13:U:102:SPO:H362	1.84	0.59
8:U:101:BCL:H2A	13:U:104:SPO:H25	1.83	0.59
6:X:25:PHE:HA	6:X:28:MET:HE2	1.83	0.59
4:I:10:ILE:HA	5:J:9:TYR:HB2	1.85	0.59
2:M:182:HIS:O	2:M:186:THR:HG23	2.02	0.58
4:O:14:ARG:O	4:O:18:VAL:HG23	2.03	0.58
8:J:102:BCL:H52	13:J:103:SPO:H243	1.84	0.58
1:L:168:HIS:CD2	2:M:183:LEU:HB3	2.39	0.58
5:C:10:THR:HG23	5:C:12:LEU:H	1.68	0.58
5:0:49:PHE:CE2	13:0:101:SPO:H11	2.39	0.58
1:L:149:GLY:O	1:L:153:HIS:ND1	2.30	0.57
2:M:197:PHE:CE1	8:M:402:BCL:HMC2	2.39	0.57
10:H:301:PC1:H111	10:H:301:PC1:H32	1.85	0.57
8:A:101:BCL:H43	13:0:101:SPO:H32	1.87	0.57
5:E:46:ARG:CZ	4:F:53:ARG:HD3	2.34	0.57
4:A:35:LEU:HD11	8:A:103:BCL:HHD	1.85	0.56
8:O:103:BCL:H172	13:P:101:SPO:H14	1.86	0.56
2:M:301:HIS:CD2	10:H:301:PC1:H11	2.40	0.56
13:3:102:SPO:H301	5:Z:24:TYR:HA	1.88	0.56
13:J:103:SPO:H15	5:N:42:VAL:HG23	1.88	0.56
13:J:103:SPO:H16	5:N:38:ALA:HB1	1.88	0.56
4:K:6:LYS:HB3	13:O:102:SPO:H392	1.86	0.56
4:K:38:THR:OG1	4:K:40:SER:O	2.17	0.56
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.88	0.56
2:M:53:GLY:O	2:M:57:VAL:HG23	2.06	0.56
5:N:7:LEU:HD13	5:N:9:TYR:HE2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:6:LYS:HD3	13:U:102:SPO:H403	1.87	0.55
10:D:104:PC1:H231	4:F:18:VAL:HG22	1.87	0.55
4:U:10:ILE:HD11	13:W:103:SPO:H361	1.89	0.55
8:7:101:BCL:H2	13:8:102:SPO:H243	1.87	0.55
5:P:46:ARG:HG3	4:Q:53:ARG:NH2	2.22	0.55
8:7:101:BCL:HMA2	13:X:101:SPO:H11	1.89	0.55
13:G:101:SPO:H402	13:J:101:SPO:H26	1.88	0.55
14:H:304:CDL:H741	4:F:33:LEU:HD12	1.87	0.55
13:I:102:SPO:H352	5:N:20:LEU:HG	1.89	0.55
8:7:101:BCL:HED1	8:8:101:BCL:H12	1.88	0.55
4:A:40:SER:O	5:B:46:ARG:NH1	2.40	0.55
8:7:101:BCL:CMA	13:X:101:SPO:H11	2.37	0.55
4:1:26:LEU:O	4:1:30:MET:HG2	2.08	0.54
4:3:4:PHE:O	4:3:7:ILE:HG12	2.05	0.54
2:M:205:SER:O	2:M:276:VAL:HG23	2.08	0.54
8:A:103:BCL:H12	13:B:101:SPO:H16	1.89	0.54
4:U:6:LYS:HD3	13:W:103:SPO:H393	1.90	0.54
1:L:45:GLY:HA3	9:L:303:BPB:H9B	1.90	0.54
13:V:101:SPO:H26	8:W:102:BCL:HED3	1.90	0.54
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.43	0.54
5:E:40:LEU:O	5:E:44:ILE:HG12	2.07	0.54
4:1:3:LYS:H	4:1:3:LYS:HD2	1.73	0.54
1:L:255:TRP:NE1	1:L:257:ASP:O	2.42	0.53
4:Q:38:THR:HG21	4:S:44:LEU:HD13	1.90	0.53
1:L:168:HIS:HD2	2:M:183:LEU:HB3	1.74	0.53
5:R:32:SER:O	5:R:36:ILE:HG13	2.08	0.53
9:M:403:BPB:H55	9:M:403:BPB:HHD	1.91	0.53
4:F:41:TYR:CE1	5:G:46:ARG:HG2	2.43	0.53
5:E:7:LEU:HD21	5:G:20:LEU:HD12	1.90	0.53
10:L:304:PC1:H221	4:D:33:LEU:HD13	1.90	0.53
5:B:7:LEU:HD12	5:E:16:GLN:HB3	1.90	0.53
13:3:104:SPO:H182	13:3:104:SPO:C14	2.39	0.53
4:Q:20:GLN:OE1	5:R:24:TYR:OH	2.18	0.52
3:H:154:ARG:NH1	3:H:158:LEU:HD13	2.24	0.52
5:B:27:GLY:HA3	13:B:101:SPO:H26	1.91	0.52
1:L:36:VAL:HG22	11:M:404:U10:H403	1.91	0.52
3:H:226:THR:O	3:H:230:GLU:HG3	2.09	0.52
13:T:102:SPO:H11	13:T:102:SPO:H81	1.91	0.52
4:7:13:PRO:HB3	5:8:20:LEU:HD21	1.91	0.52
8:S:102:BCL:HMA2	13:T:101:SPO:H11	1.92	0.52
5:8:6:ASP:OD1	5:8:6:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:8:7:LEU:HB2	13:9:102:SPO:H403	1.92	0.52
2:M:123:PHE:HB2	13:M:405:SPO:H32	1.91	0.51
1:L:133:LEU:HD21	6:X:45:ILE:HD11	1.92	0.51
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.92	0.51
4:3:5:TYR:HB2	5:Z:17:ALA:HB1	1.92	0.51
3:H:191:LEU:HD11	3:H:213:PHE:HE2	1.75	0.51
5:R:10:THR:HG23	5:R:12:LEU:H	1.75	0.51
2:M:63:GLY:HA3	9:M:403:BPB:H5A	1.91	0.51
4:A:22:VAL:HA	10:A:102:PC1:H2F2	1.92	0.51
13:I:102:SPO:H16	8:N:101:BCL:O1A	2.10	0.51
2:M:261:THR:HG22	2:M:262:MET:H	1.76	0.51
13:T:102:SPO:H182	13:T:102:SPO:H14	1.92	0.51
4:W:29:VAL:HG11	10:W:101:PC1:H3A1	1.93	0.51
4:7:14:ARG:HG2	6:X:22:TRP:CZ2	2.46	0.50
3:H:54:GLY:H	10:A:104:PC1:H131	1.76	0.50
3:H:52:ASN:HA	10:A:104:PC1:H143	1.94	0.50
5:2:32:SER:O	5:2:36:ILE:HG12	2.12	0.50
8:U:101:BCL:HBA1	13:U:104:SPO:H27	1.94	0.50
5:C:46:ARG:NH1	4:3:53:ARG:HD3	2.27	0.49
8:A:103:BCL:HBB3	8:D:101:BCL:CHC	2.42	0.49
10:A:104:PC1:H351	8:D:101:BCL:H72	1.94	0.49
4:3:6:LYS:HA	4:3:9:MET:HG2	1.94	0.49
4:3:26:LEU:HD21	7:Y:42:VAL:HG21	1.94	0.49
5:J:30:LEU:O	5:J:34:VAL:HG23	2.13	0.49
3:H:105:MET:HE2	3:H:243:TYR:HB2	1.95	0.49
8:S:102:BCL:CMA	13:T:101:SPO:H11	2.42	0.49
7:Y:48:ALA:HA	11:Y:501:U10:H101	1.94	0.49
2:M:240:ASP:O	3:H:117:ARG:NH2	2.32	0.49
13:F:102:SPO:H311	5:G:23:VAL:HG12	1.95	0.49
13:F:102:SPO:H16	8:F:103:BCL:H12	1.94	0.49
5:B:15:GLU:OE2	5:B:15:GLU:HA	2.12	0.49
13:U:102:SPO:H133	8:W:102:BCL:HBA2	1.95	0.49
1:L:241:VAL:HG21	9:L:303:BPB:H55	1.95	0.48
5:E:49:PHE:HB3	13:E:102:SPO:C8	2.43	0.48
4:7:30:MET:O	4:7:34:ILE:HG12	2.13	0.48
1:L:253:THR:HA	6:X:57:ILE:HD11	1.95	0.48
4:A:16:VAL:HG22	10:A:104:PC1:H11	1.94	0.48
13:I:102:SPO:H132	13:I:102:SPO:H10	1.50	0.48
4:Q:4:PHE:O	4:Q:7:ILE:HG22	2.13	0.48
2:M:261:THR:HG22	2:M:262:MET:N	2.29	0.48
5:E:21:HIS:O	5:E:25:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:8:31:PHE:CE1	8:8:101:BCL:H2	2.49	0.48
8:N:101:BCL:H72	8:N:101:BCL:H2	1.96	0.48
13:O:102:SPO:H11	8:O:103:BCL:CMA	2.44	0.48
8:L:302:BCL:HMD2	8:M:402:BCL:HBB3	1.96	0.48
13:B:101:SPO:H402	4:9:6:LYS:HB3	1.94	0.48
1:L:211:HIS:NE2	2:M:22:GLU:OE2	2.28	0.48
13:O:104:SPO:H301	5:R:24:TYR:HA	1.96	0.48
8:0:102:BCL:HMB1	8:0:102:BCL:HBB2	1.96	0.47
6:X:20:ARG:HH21	13:X:101:SPO:H352	1.79	0.47
5:T:23:VAL:HG12	13:T:101:SPO:H311	1.96	0.47
5:N:29:TRP:HA	5:N:29:TRP:CE3	2.50	0.47
4:W:6:LYS:HD3	13:3:102:SPO:H403	1.95	0.47
4:W:46:ILE:HD11	5:C:45:TRP:CZ2	2.49	0.47
13:3:102:SPO:H241	13:3:102:SPO:H26	1.06	0.47
13:3:104:SPO:H10	13:3:104:SPO:H133	1.43	0.47
10:H:301:PC1:H252	10:H:301:PC1:H281	1.81	0.47
13:G:101:SPO:C26	8:I:101:BCL:HED3	2.44	0.47
4:9:24:LEU:HB2	8:9:101:BCL:H42	1.96	0.47
1:L:249:ILE:O	1:L:253:THR:OG1	2.32	0.47
3:H:53:GLN:H	10:A:104:PC1:H143	1.80	0.47
3:H:154:ARG:HH11	3:H:158:LEU:HD13	1.79	0.47
13:V:101:SPO:H133	13:V:101:SPO:H10	1.44	0.47
4:A:15:ARG:HD3	10:A:102:PC1:H121	1.96	0.47
8:J:102:BCL:H162	8:J:102:BCL:H192	1.68	0.47
4:W:8:TRP:O	5:C:10:THR:HG21	2.15	0.47
10:D:104:PC1:H271	8:F:101:BCL:H72	1.97	0.47
13:I:102:SPO:H27	5:N:24:TYR:CD2	2.50	0.47
4:A:19:ALA:HB2	10:A:102:PC1:H341	1.97	0.47
13:F:102:SPO:H132	13:F:102:SPO:H10	1.66	0.47
13:F:102:SPO:H312	13:F:102:SPO:H291	1.75	0.47
5:J:46:ARG:NH1	4:K:53:ARG:HD3	2.29	0.47
13:I:102:SPO:H11	8:N:101:BCL:CMA	2.45	0.46
13:J:103:SPO:H183	13:J:103:SPO:C14	2.44	0.46
13:N:102:SPO:H183	5:P:38:ALA:HB1	1.98	0.46
13:3:102:SPO:H11	8:3:103:BCL:CMA	2.45	0.46
8:R:101:BCL:H152	13:T:102:SPO:H183	1.98	0.46
4:1:3:LYS:HB3	4:1:5:TYR:CE1	2.50	0.46
3:H:228:LEU:HG	3:H:232:LYS:HE2	1.98	0.46
8:A:103:BCL:H192	8:A:103:BCL:H162	1.72	0.46
10:D:104:PC1:H153	4:F:14:ARG:HB3	1.97	0.46
13:G:101:SPO:H182	13:G:101:SPO:H15	1.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:17:PHE:CE2	6:X:23:VAL:HG22	2.50	0.46
1:L:31:VAL:HG13	1:L:31:VAL:O	2.15	0.46
10:D:104:PC1:H111	10:D:104:PC1:H152	1.69	0.46
4:K:10:ILE:HG22	5:N:9:TYR:HD2	1.80	0.46
5:8:26:SER:HB3	6:X:20:ARG:HH22	1.80	0.46
3:H:170:ASP:HB2	3:H:177:ARG:HG3	1.98	0.46
13:I:102:SPO:H302	5:N:24:TYR:HA	1.97	0.46
5:R:49:PHE:CD2	8:R:101:BCL:H18	2.50	0.46
10:L:306:PC1:H3A2	10:L:306:PC1:H372	1.53	0.46
13:0:101:SPO:H133	8:0:102:BCL:H141	1.97	0.46
5:E:21:HIS:HE1	8:F:101:BCL:H193	1.80	0.46
13:T:102:SPO:H131	13:T:102:SPO:H15	1.59	0.46
4:W:6:LYS:HG2	4:W:9:MET:HG3	1.98	0.46
8:7:101:BCL:H102	5:8:39:HIS:CD2	2.50	0.46
8:L:302:BCL:HMB1	8:L:302:BCL:HBB2	1.98	0.46
8:F:103:BCL:H51	13:G:101:SPO:H243	1.98	0.46
13:O:102:SPO:H10	13:O:102:SPO:H132	1.49	0.46
13:P:101:SPO:H27	8:Q:101:BCL:HED3	1.97	0.46
14:H:304:CDL:H331	14:H:304:CDL:H362	1.49	0.45
5:B:5:SER:OG	5:B:6:ASP:N	2.49	0.45
13:D:103:SPO:H23	13:D:103:SPO:H5	1.62	0.45
4:O:34:ILE:O	4:O:38:THR:HG23	2.16	0.45
3:H:1:MET:HG2	3:H:12:LEU:HD12	1.98	0.45
8:A:103:BCL:CMA	13:B:101:SPO:H11	2.47	0.45
4:A:42:ASN:O	4:A:46:ILE:HG13	2.16	0.45
13:O:102:SPO:H22A	4:Q:32:HIS:HB3	1.98	0.45
8:O:103:BCL:H203	13:P:101:SPO:H11	1.98	0.45
4:Q:11:PHE:HE2	4:S:17:PHE:HD2	1.64	0.45
13:3:102:SPO:H343	13:3:102:SPO:H311	1.78	0.45
10:H:302:PC1:H362	10:H:302:PC1:H251	1.97	0.45
8:A:103:BCL:H102	8:A:103:BCL:HMB2	1.99	0.45
8:0:102:BCL:H61	8:0:102:BCL:H2	1.80	0.45
13:T:102:SPO:H182	13:T:102:SPO:C14	2.47	0.45
5:2:14:ASP:OD1	5:2:14:ASP:N	2.47	0.45
5:B:13:THR:OG1	5:B:16:GLN:HG3	2.16	0.45
4:I:23:PHE:HE1	4:K:25:PHE:CE1	2.35	0.45
4:Q:35:LEU:HD11	8:R:101:BCL:HHD	1.98	0.45
13:G:101:SPO:H20	13:G:101:SPO:H181	1.33	0.45
7:Y:6:GLU:O	7:Y:10:ARG:HG2	2.16	0.45
13:F:102:SPO:H15	13:F:102:SPO:H182	1.45	0.45
13:9:102:SPO:H10	13:9:102:SPO:H132	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:276:PRO:HD2	10:W:101:PC1:H142	1.99	0.45
14:M:406:CDL:H821	14:M:406:CDL:H851	1.71	0.45
13:N:102:SPO:H403	4:O:20:GLN:NE2	2.31	0.45
5:T:27:GLY:HA3	13:T:101:SPO:H26	1.99	0.45
13:M:405:SPO:H132	13:M:405:SPO:H10	1.46	0.45
14:H:304:CDL:H311	14:H:304:CDL:HA61	1.92	0.45
10:A:104:PC1:H153	4:D:14:ARG:HB3	1.99	0.45
13:B:101:SPO:H312	13:B:101:SPO:H291	1.72	0.45
13:T:102:SPO:H291	13:T:102:SPO:H311	1.11	0.45
4:W:33:LEU:HD21	10:W:101:PC1:H361	1.98	0.45
13:0:101:SPO:H131	13:0:101:SPO:H15	1.59	0.45
13:N:102:SPO:H403	4:O:20:GLN:HE21	1.82	0.44
4:1:41:TYR:OH	5:2:48:TRP:HB3	2.17	0.44
1:L:182:THR:HG21	11:L:305:U10:H18	1.99	0.44
5:N:49:PHE:CD2	13:N:102:SPO:H9	2.52	0.44
4:7:35:LEU:HD11	8:7:101:BCL:HHD	1.99	0.44
8:E:101:BCL:HMB1	8:E:101:BCL:HBB2	1.99	0.44
13:F:102:SPO:H26	5:G:27:GLY:HA3	1.99	0.44
13:T:102:SPO:H10	13:T:102:SPO:H132	1.37	0.44
4:U:6:LYS:HB2	13:W:103:SPO:H351	1.99	0.44
1:L:172:ALA:HB3	1:L:247:CYS:HB3	1.98	0.44
8:L:307:BCL:H101	8:L:307:BCL:H13	1.61	0.44
8:N:101:BCL:H141	8:N:101:BCL:H162	1.82	0.44
13:0:101:SPO:H291	13:0:101:SPO:H312	1.26	0.44
11:L:305:U10:H71	11:L:305:U10:H1M1	1.75	0.44
14:M:406:CDL:H211	14:M:406:CDL:H241	1.53	0.44
1:L:224:ILE:HG22	11:L:305:U10:H8	2.00	0.44
8:U:103:BCL:HBB2	8:U:103:BCL:HMB1	1.99	0.44
4:3:36:LEU:O	4:3:42:ASN:ND2	2.45	0.44
13:B:101:SPO:H403	4:9:10:ILE:HD11	2.00	0.44
13:O:102:SPO:H15	13:O:102:SPO:H182	1.50	0.44
13:V:101:SPO:H81	5:C:45:TRP:HB2	1.99	0.44
8:1:102:BCL:H91	8:1:102:BCL:H112	1.80	0.44
4:A:12:ASP:OD2	4:A:13:PRO:HD2	2.17	0.44
5:G:49:PHE:CZ	13:G:101:SPO:H11	2.52	0.44
4:O:41:TYR:CE1	5:P:46:ARG:HG2	2.52	0.44
13:M:405:SPO:H312	13:M:405:SPO:H291	1.44	0.44
3:H:106:LYS:HD2	3:H:106:LYS:HA	1.80	0.44
8:W:102:BCL:OBB	8:W:102:BCL:HHC	2.18	0.44
4:9:35:LEU:HD11	8:0:102:BCL:HHD	1.99	0.44
1:L:219:LEU:HD11	2:M:133:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:101:SPO:H182	13:B:101:SPO:H15	1.58	0.43
13:J:101:SPO:H11	8:J:102:BCL:CMA	2.48	0.43
4:O:12:ASP:HB3	4:O:15:ARG:HD3	2.00	0.43
1:L:49:ILE:HD13	1:L:66:VAL:HG21	2.00	0.43
9:M:403:BPB:H6	9:M:403:BPB:H4	1.81	0.43
13:D:102:SPO:H132	13:D:102:SPO:H10	1.63	0.43
5:G:7:LEU:HD21	5:J:12:LEU:HD11	1.99	0.43
5:N:49:PHE:CG	13:N:102:SPO:H9	2.53	0.43
13:V:101:SPO:H15	13:V:101:SPO:H182	1.59	0.43
8:7:101:BCL:H61	8:7:101:BCL:H41	1.82	0.43
7:Y:7:PHE:HE1	11:Y:501:U10:H103	1.83	0.43
1:L:22:PHE:O	1:L:32:GLY:HA2	2.17	0.43
2:M:241:ARG:NH1	3:H:38:GLU:OE1	2.42	0.43
13:D:102:SPO:H26	13:D:103:SPO:H37	2.00	0.43
8:O:103:BCL:HMB1	8:O:103:BCL:HBB2	2.00	0.43
13:W:103:SPO:H343	13:W:103:SPO:H312	1.65	0.43
13:X:101:SPO:H132	13:X:101:SPO:H10	1.48	0.43
1:L:168:HIS:ND1	8:L:301:BCL:HMC2	2.33	0.43
13:M:405:SPO:H342	13:M:405:SPO:H311	1.77	0.43
3:H:163:LYS:NZ	3:H:182:GLU:OE2	2.52	0.43
4:A:18:VAL:HG22	10:A:102:PC1:H251	2.00	0.43
8:F:103:BCL:HMB1	8:F:103:BCL:HBB2	2.00	0.43
8:R:101:BCL:H162	8:R:101:BCL:H141	1.74	0.43
5:T:13:THR:OG1	5:T:16:GLN:HG3	2.18	0.43
13:3:102:SPO:H311	13:3:102:SPO:H292	1.53	0.43
13:9:102:SPO:H15	13:9:102:SPO:H182	1.52	0.43
8:L:302:BCL:HBB3	9:L:303:BPB:H14	2.00	0.43
13:D:103:SPO:H20	13:D:103:SPO:H181	1.21	0.43
8:R:101:BCL:HMB1	8:R:101:BCL:HBB2	2.00	0.43
4:U:12:ASP:N	5:V:10:THR:HG21	2.34	0.43
13:V:101:SPO:HM13	13:V:101:SPO:H41	1.65	0.43
4:9:41:TYR:H	4:9:46:ILE:HD11	1.83	0.43
2:M:271:TRP:HA	2:M:274:VAL:HG22	2.01	0.43
14:H:304:CDL:H791	14:H:304:CDL:H822	1.83	0.43
13:I:102:SPO:H182	13:I:102:SPO:H15	1.48	0.43
8:N:101:BCL:HMB1	8:N:101:BCL:HBB2	2.00	0.43
5:T:35:ALA:O	5:T:39:HIS:ND1	2.44	0.43
4:U:38:THR:HG21	4:W:44:LEU:HD13	2.00	0.43
4:W:6:LYS:CD	13:3:102:SPO:H403	2.48	0.43
13:9:102:SPO:H26	5:0:27:GLY:HA3	2.00	0.43
4:A:25:PHE:CD2	10:A:102:PC1:H2F1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:102:SPO:H11	8:E:101:BCL:HMA2	2.00	0.43
13:O:104:SPO:H291	13:O:104:SPO:H312	1.37	0.43
9:M:403:BPB:HMB	9:M:403:BPB:HBBB	2.01	0.43
5:E:8:GLY:C	5:E:10:THR:H	2.22	0.43
4:K:3:LYS:HD2	4:K:6:LYS:HE3	2.01	0.43
8:R:101:BCL:H162	8:R:101:BCL:H192	1.68	0.43
5:V:19:GLU:HG3	5:V:20:LEU:N	2.33	0.43
5:8:20:LEU:HD13	6:X:19:LEU:HD11	2.00	0.43
13:8:102:SPO:H5	13:8:102:SPO:H21A	1.68	0.43
6:X:49:ARG:O	6:X:53:ARG:HG2	2.19	0.43
11:L:305:U10:H152	11:L:305:U10:H101	2.01	0.43
10:L:306:PC1:H351	10:L:306:PC1:H381	1.92	0.43
2:M:158:MET:HE3	2:M:162:PHE:HB3	2.01	0.43
13:N:102:SPO:H15	13:N:102:SPO:H182	1.23	0.43
4:O:3:LYS:HE3	4:O:6:LYS:HD2	2.01	0.43
2:M:103:LEU:HD11	2:M:166:ILE:HA	2.01	0.42
5:C:35:ALA:O	5:C:39:HIS:ND1	2.52	0.42
13:3:104:SPO:H291	13:3:104:SPO:H312	1.37	0.42
8:9:101:BCL:HHD	5:0:42:VAL:HG21	2.01	0.42
3:H:170:ASP:OD1	3:H:172:PRO:HD2	2.18	0.42
3:H:171:ILE:HB	3:H:172:PRO:HD3	2.02	0.42
10:D:104:PC1:H262	10:D:104:PC1:H232	1.41	0.42
6:X:16:LYS:O	6:X:20:ARG:HG3	2.19	0.42
2:M:86:LEU:HD23	2:M:86:LEU:HA	1.83	0.42
2:M:241:ARG:HD3	3:H:38:GLU:OE1	2.19	0.42
13:D:103:SPO:H131	13:D:103:SPO:C18	2.47	0.42
8:1:101:BCL:HHC	8:1:101:BCL:OBB	2.19	0.42
6:X:57:ILE:HG22	6:X:61:GLN:NE2	2.34	0.42
2:M:249:ALA:HB1	2:M:259:ASN:ND2	2.35	0.42
5:E:49:PHE:HB3	13:E:102:SPO:H81	2.00	0.42
4:I:35:LEU:HD11	8:J:102:BCL:HHD	2.01	0.42
8:J:102:BCL:HBB2	8:J:102:BCL:HMB1	2.01	0.42
13:J:103:SPO:H391	4:K:17:PHE:HB3	2.02	0.42
8:S:102:BCL:HMB1	8:S:102:BCL:HBB2	2.02	0.42
5:R:40:LEU:O	5:R:44:ILE:HG12	2.20	0.42
13:T:101:SPO:H132	13:T:101:SPO:H10	1.59	0.42
8:3:101:BCL:C1D	13:3:104:SPO:H181	2.50	0.42
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.01	0.42
2:M:81:ASN:HB3	2:M:84:VAL:HB	2.00	0.42
2:M:227:SER:HA	2:M:231:GLY:H	1.84	0.42
4:O:30:MET:O	4:O:34:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:101:BCL:H192	8:7:101:BCL:H162	1.79	0.42
8:8:101:BCL:H92	8:8:101:BCL:H62	1.75	0.42
2:M:39:LEU:O	2:M:43:GLY:N	2.45	0.42
13:O:102:SPO:H42	8:Q:101:BCL:HMB2	2.02	0.42
8:S:101:BCL:H41	13:T:102:SPO:H37	2.01	0.42
13:8:102:SPO:H242	13:8:102:SPO:C28	2.49	0.42
7:Y:13:MET:HA	7:Y:16:VAL:HG22	2.01	0.42
14:M:406:CDL:H781	14:M:406:CDL:H811	1.84	0.42
4:I:13:PRO:HB3	5:J:20:LEU:HD11	2.02	0.42
5:T:20:LEU:HA	13:T:101:SPO:H361	2.02	0.42
8:7:101:BCL:HMB1	8:7:101:BCL:HBB2	2.02	0.42
6:X:59:GLU:OE1	6:X:59:GLU:N	2.53	0.42
11:L:308:U10:H13	11:L:308:U10:H172	1.80	0.42
13:F:102:SPO:H312	13:F:102:SPO:H343	1.76	0.42
8:U:101:BCL:HHC	8:U:101:BCL:OBB	2.20	0.42
5:2:30:LEU:O	5:2:34:VAL:HG23	2.20	0.42
1:L:35:GLY:HA2	1:L:103:ARG:HD2	2.01	0.42
1:L:117:ILE:HB	1:L:118:PRO:HD3	2.02	0.42
13:E:102:SPO:H241	13:E:102:SPO:H26	1.08	0.42
13:U:102:SPO:H291	13:U:102:SPO:H312	1.21	0.42
13:9:102:SPO:H26	5:0:27:GLY:C	2.40	0.42
2:M:235:LEU:HD12	2:M:235:LEU:HA	1.94	0.41
3:H:89:ARG:NH2	3:H:92:VAL:O	2.54	0.41
8:A:103:BCL:O1A	13:B:101:SPO:H16	2.20	0.41
8:J:102:BCL:H162	8:J:102:BCL:H141	1.74	0.41
13:U:104:SPO:H241	13:U:104:SPO:H26	1.16	0.41
8:8:101:BCL:H8	8:8:101:BCL:H121	1.75	0.41
4:9:27:LEU:O	4:9:31:ILE:HG13	2.20	0.41
1:L:226:THR:O	1:L:229:ILE:HG22	2.21	0.41
8:A:103:BCL:H162	8:A:103:BCL:H141	1.77	0.41
1:L:108:CYS:HG	2:M:251:PHE:HE2	1.68	0.41
13:M:405:SPO:H181	13:M:405:SPO:H20	1.86	0.41
13:B:101:SPO:H10	13:B:101:SPO:H132	1.50	0.41
8:F:101:BCL:HHC	8:F:101:BCL:OBB	2.20	0.41
8:U:103:BCL:H2	8:U:103:BCL:C7	2.44	0.41
3:H:52:ASN:ND2	10:H:302:PC1:H142	2.35	0.41
13:V:101:SPO:H341	13:V:101:SPO:H362	1.19	0.41
13:V:101:SPO:C37	13:W:103:SPO:H26	2.50	0.41
13:3:104:SPO:H312	13:3:104:SPO:H343	1.78	0.41
13:P:101:SPO:H15	13:P:101:SPO:H183	1.60	0.41
8:S:102:BCL:H2	8:S:102:BCL:C7	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:102:BCL:HMA1	8:U:101:BCL:HMA1	2.03	0.41
4:1:28:ALA:O	4:1:32:HIS:ND1	2.50	0.41
13:X:101:SPO:H182	13:X:101:SPO:H15	1.49	0.41
2:M:277:THR:OG1	9:M:403:BPB:HAC	2.21	0.41
13:M:405:SPO:H19	13:M:405:SPO:H22	1.54	0.41
5:G:40:LEU:O	5:G:44:ILE:HG12	2.19	0.41
4:I:7:ILE:HD12	4:I:10:ILE:HD11	2.01	0.41
5:J:19:GLU:O	5:J:23:VAL:HG12	2.21	0.41
5:C:49:PHE:HE2	8:C:101:BCL:H162	1.85	0.41
4:7:20:GLN:NE2	5:8:24:TYR:OH	2.41	0.41
1:L:207:ARG:HG3	2:M:142:MET:HG2	2.03	0.41
2:M:261:THR:HG23	3:H:38:GLU:HG3	2.01	0.41
3:H:122:GLU:HB2	3:H:227:LEU:HD21	2.03	0.41
10:A:102:PC1:H291	13:0:101:SPO:H393	2.03	0.41
5:N:29:TRP:HA	5:N:29:TRP:HE3	1.84	0.41
2:M:16:ALA:HB1	2:M:32:VAL:HG11	2.02	0.41
13:W:103:SPO:C32	13:W:103:SPO:H291	2.51	0.41
4:7:25:PHE:CZ	6:X:35:GLY:HA2	2.56	0.41
4:7:38:THR:HG21	4:9:44:LEU:HD13	2.03	0.41
6:X:37:VAL:O	6:X:41:THR:HG23	2.20	0.41
1:L:199:ASN:HB3	14:M:406:CDL:HB21	2.03	0.41
13:D:103:SPO:H182	13:D:103:SPO:H15	1.35	0.41
4:K:28:ALA:O	4:K:32:HIS:ND1	2.51	0.41
4:W:33:LEU:HD13	10:W:101:PC1:H252	2.02	0.41
13:3:102:SPO:H183	13:3:102:SPO:H15	1.51	0.41
11:L:305:U10:H101	11:L:305:U10:C15	2.51	0.41
13:D:103:SPO:H14	5:E:42:VAL:CG2	2.51	0.41
5:R:19:GLU:O	5:R:23:VAL:HG23	2.21	0.41
4:1:43:TRP:HA	4:1:46:ILE:HG12	2.03	0.41
8:9:101:BCL:HHC	8:9:101:BCL:OBB	2.21	0.41
1:L:170:ASN:HB3	1:L:173:HIS:HB2	2.02	0.40
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.55	0.40
4:A:33:LEU:HD23	4:A:33:LEU:HA	1.93	0.40
4:K:12:ASP:HB3	4:K:15:ARG:HD2	2.02	0.40
10:W:101:PC1:H272	10:W:101:PC1:H241	1.81	0.40
5:8:40:LEU:HD23	5:8:40:LEU:HA	1.97	0.40
11:M:404:U10:H251	11:M:404:U10:H272	1.93	0.40
3:H:211:ASP:N	3:H:211:ASP:OD1	2.54	0.40
5:B:12:LEU:HD23	5:B:12:LEU:HA	1.89	0.40
5:B:40:LEU:O	5:B:44:ILE:HD12	2.21	0.40
13:J:103:SPO:C16	5:N:38:ALA:HB1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:9:MET:HE1	5:C:14:ASP:HA	2.03	0.40
1:L:193:LEU:HD22	1:L:216:PHE:CE2	2.56	0.40
14:H:304:CDL:H332	14:H:304:CDL:H512	2.03	0.40
4:D:51:TYR:O	4:D:53:ARG:N	2.53	0.40
4:F:12:ASP:HB3	4:F:15:ARG:HG3	2.03	0.40
8:S:101:BCL:H52	13:T:102:SPO:H362	2.03	0.40
8:U:101:BCL:H43	13:U:104:SPO:H32	2.03	0.40
4:7:35:LEU:HD23	4:7:35:LEU:HA	1.94	0.40
6:X:21:LEU:HD12	6:X:21:LEU:HA	1.81	0.40
8:L:301:BCL:HHC	8:L:301:BCL:OBB	2.22	0.40
2:M:196:LEU:HD12	2:M:196:LEU:HA	1.87	0.40
2:M:249:ALA:HB1	2:M:259:ASN:HD22	1.85	0.40
4:Q:8:TRP:O	5:R:10:THR:HG21	2.21	0.40
4:7:32:HIS:NE2	8:7:101:BCL:HMD1	2.37	0.40
13:0:101:SPO:H20	13:0:101:SPO:H181	1.19	0.40
6:X:19:LEU:O	6:X:23:VAL:HG23	2.20	0.40
1:L:195:LEU:HD11	2:M:267:ARG:HA	2.04	0.40
1:L:235:LEU:HD12	2:M:42:PHE:CZ	2.57	0.40
8:L:302:BCL:O1D	10:H:301:PC1:H282	2.21	0.40
9:L:303:BPB:HBBB	9:L:303:BPB:HMB	2.02	0.40
13:D:102:SPO:H291	13:D:102:SPO:H312	1.50	0.40
13:D:103:SPO:H14	5:E:42:VAL:HG23	2.04	0.40
13:J:103:SPO:H312	13:J:103:SPO:H343	1.73	0.40
13:O:104:SPO:H133	13:O:104:SPO:H10	1.63	0.40
4:U:17:PHE:CZ	13:U:102:SPO:H32	2.57	0.40
4:W:36:LEU:O	4:W:42:ASN:ND2	2.54	0.40
5:8:31:PHE:HB2	13:X:101:SPO:H242	2.03	0.40
13:8:102:SPO:H291	13:8:102:SPO:H311	1.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/282 (99%)	267 (96%)	12 (4%)	0	100	100
2	M	303/308 (98%)	296 (98%)	7 (2%)	0	100	100
3	H	245/260 (94%)	240 (98%)	5 (2%)	0	100	100
4	1	51/58 (88%)	48 (94%)	3 (6%)	0	100	100
4	3	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	7	44/58 (76%)	43 (98%)	1 (2%)	0	100	100
4	9	52/58 (90%)	52 (100%)	0	0	100	100
4	A	52/58 (90%)	52 (100%)	0	0	100	100
4	D	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	F	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	I	52/58 (90%)	52 (100%)	0	0	100	100
4	K	52/58 (90%)	52 (100%)	0	0	100	100
4	O	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	Q	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	S	52/58 (90%)	52 (100%)	0	0	100	100
4	U	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	W	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
5	0	42/49 (86%)	42 (100%)	0	0	100	100
5	2	37/49 (76%)	37 (100%)	0	0	100	100
5	8	42/49 (86%)	42 (100%)	0	0	100	100
5	B	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
5	C	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	E	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	G	41/49 (84%)	41 (100%)	0	0	100	100
5	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	N	41/49 (84%)	41 (100%)	0	0	100	100
5	P	41/49 (84%)	41 (100%)	0	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	41/49 (84%)	41 (100%)	0	0	100	100
5	V	41/49 (84%)	41 (100%)	0	0	100	100
5	Z	40/49 (82%)	40 (100%)	0	0	100	100
6	X	50/82 (61%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Y	48/53 (91%)	48 (100%)	0	0	100	100
All	All	2217/2483 (89%)	2173 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/221 (100%)	220 (100%)	0	100	100
2	M	239/241 (99%)	237 (99%)	2 (1%)	81	94
3	H	199/208 (96%)	198 (100%)	1 (0%)	88	96
4	1	48/51 (94%)	47 (98%)	1 (2%)	53	84
4	3	49/51 (96%)	48 (98%)	1 (2%)	55	84
4	7	43/51 (84%)	43 (100%)	0	100	100
4	9	49/51 (96%)	49 (100%)	0	100	100
4	A	49/51 (96%)	48 (98%)	1 (2%)	55	84
4	D	49/51 (96%)	49 (100%)	0	100	100
4	F	49/51 (96%)	48 (98%)	1 (2%)	55	84
4	I	49/51 (96%)	49 (100%)	0	100	100
4	K	49/51 (96%)	47 (96%)	2 (4%)	30	64
4	O	49/51 (96%)	47 (96%)	2 (4%)	30	64
4	Q	49/51 (96%)	48 (98%)	1 (2%)	55	84
4	S	49/51 (96%)	47 (96%)	2 (4%)	30	64
4	U	49/51 (96%)	48 (98%)	1 (2%)	55	84
4	W	49/51 (96%)	48 (98%)	1 (2%)	55	84
5	0	36/40 (90%)	35 (97%)	1 (3%)	43	77
5	2	32/40 (80%)	32 (100%)	0	100	100
5	8	36/40 (90%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	B	37/40 (92%)	37 (100%)	0	100 100
5	C	35/40 (88%)	35 (100%)	0	100 100
5	E	35/40 (88%)	34 (97%)	1 (3%)	42 76
5	G	35/40 (88%)	35 (100%)	0	100 100
5	J	35/40 (88%)	35 (100%)	0	100 100
5	N	35/40 (88%)	34 (97%)	1 (3%)	42 76
5	P	35/40 (88%)	35 (100%)	0	100 100
5	R	35/40 (88%)	34 (97%)	1 (3%)	42 76
5	T	35/40 (88%)	35 (100%)	0	100 100
5	V	35/40 (88%)	35 (100%)	0	100 100
5	Z	34/40 (85%)	34 (100%)	0	100 100
6	X	40/66 (61%)	39 (98%)	1 (2%)	47 80
7	Y	34/37 (92%)	34 (100%)	0	100 100
All	All	1901/2047 (93%)	1880 (99%)	21 (1%)	74 92

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	104	SER
2	M	240	ASP
3	H	93	SER
4	A	37	SER
5	E	22	SER
4	F	1	MET
4	K	1	MET
4	K	14	ARG
5	N	26	SER
4	O	5	TYR
4	O	20	GLN
4	Q	9	MET
5	R	22	SER
4	S	3	LYS
4	S	52	ASN
4	U	1	MET
4	W	20	GLN
4	3	39	PRO
4	1	9	MET

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Mol	Chain	Res	Type
5	0	22	SER
6	X	27	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	126	HIS
5	C	16	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 76 ligands modelled in this entry, 1 is monoatomic - leaving 75 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BCL	3	103	-	58,74,74	1.24	3 (5%)	69,115,115	1.35	11 (15%)
13	SPO	U	102	-	40,41,41	3.35	21 (52%)	47,50,50	10.13	29 (61%)
13	SPO	X	101	-	37,38,41	3.43	21 (56%)	43,46,50	10.84	29 (67%)
8	BCL	R	101	-	58,74,74	1.21	3 (5%)	69,115,115	1.55	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	PC1	H	302	-	41,41,53	1.35	6 (14%)	47,49,61	1.20	4 (8%)
13	SPO	O	102	-	40,41,41	3.45	20 (50%)	47,50,50	10.05	32 (68%)
11	U10	Y	501	-	38,38,63	2.69	12 (31%)	46,49,79	1.58	10 (21%)
13	SPO	M	405	-	40,41,41	3.42	21 (52%)	47,50,50	10.10	32 (68%)
8	BCL	L	307	-	58,74,74	1.21	4 (6%)	69,115,115	1.61	13 (18%)
13	SPO	I	102	-	40,41,41	3.47	21 (52%)	47,50,50	9.90	30 (63%)
8	BCL	L	302	-	55,71,74	1.24	4 (7%)	65,111,115	1.42	10 (15%)
14	CDL	M	406	-	99,99,99	1.15	6 (6%)	105,111,111	1.44	7 (6%)
8	BCL	M	402	-	58,74,74	1.20	4 (6%)	69,115,115	1.50	14 (20%)
13	SPO	3	104	-	40,41,41	3.79	21 (52%)	47,50,50	10.29	30 (63%)
10	PC1	D	104	-	36,36,53	1.41	6 (16%)	42,44,61	1.08	2 (4%)
8	BCL	L	301	-	58,74,74	1.24	4 (6%)	69,115,115	1.49	11 (15%)
13	SPO	D	102	-	40,41,41	3.40	21 (52%)	47,50,50	10.07	28 (59%)
10	PC1	L	306	-	35,35,53	1.45	7 (20%)	41,43,61	1.18	3 (7%)
8	BCL	S	101	-	58,74,74	1.23	4 (6%)	69,115,115	1.42	10 (14%)
8	BCL	E	101	-	58,74,74	1.24	3 (5%)	69,115,115	1.63	14 (20%)
11	U10	M	404	-	48,48,63	2.68	14 (29%)	58,61,79	1.62	14 (24%)
8	BCL	A	101	-	58,74,74	1.22	4 (6%)	69,115,115	1.42	10 (14%)
13	SPO	T	101	-	40,41,41	3.36	20 (50%)	47,50,50	10.29	29 (61%)
8	BCL	O	101	-	58,74,74	1.22	4 (6%)	69,115,115	1.47	10 (14%)
8	BCL	S	102	-	58,74,74	1.22	3 (5%)	69,115,115	1.54	15 (21%)
8	BCL	W	102	-	58,74,74	1.22	4 (6%)	69,115,115	1.45	12 (17%)
10	PC1	L	304	-	34,34,53	1.44	6 (17%)	40,42,61	1.16	3 (7%)
8	BCL	J	102	-	58,74,74	1.24	3 (5%)	69,115,115	1.40	12 (17%)
8	BCL	I	101	-	58,74,74	1.24	4 (6%)	69,115,115	1.41	10 (14%)
8	BCL	F	103	-	58,74,74	1.18	3 (5%)	69,115,115	1.48	13 (18%)
11	U10	L	308	-	38,38,63	2.69	12 (31%)	46,49,79	1.58	10 (21%)
8	BCL	O	103	-	58,74,74	1.24	4 (6%)	69,115,115	1.47	12 (17%)
13	SPO	W	103	-	40,41,41	3.50	22 (55%)	47,50,50	10.01	31 (65%)
11	U10	L	305	-	43,43,63	2.69	13 (30%)	52,55,79	1.68	13 (25%)
8	BCL	7	101	-	58,74,74	1.21	3 (5%)	69,115,115	1.59	13 (18%)
13	SPO	0	101	-	40,41,41	3.50	22 (55%)	47,50,50	11.31	30 (63%)
13	SPO	9	102	-	40,41,41	3.43	20 (50%)	47,50,50	10.20	28 (59%)
8	BCL	U	101	-	58,74,74	1.23	4 (6%)	69,115,115	1.43	10 (14%)
8	BCL	Q	101	-	58,74,74	1.23	4 (6%)	69,115,115	1.45	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BCL	U	103	-	58,74,74	1.24	3 (5%)	69,115,115	1.68	15 (21%)
10	PC1	A	104	-	31,31,53	1.51	6 (19%)	37,39,61	1.17	3 (8%)
10	PC1	W	101	-	36,36,53	1.45	6 (16%)	42,44,61	1.13	2 (4%)
9	BPB	L	303	-	46,67,70	1.57	2 (4%)	43,97,101	1.36	6 (13%)
13	SPO	G	101	-	40,41,41	3.59	24 (60%)	47,50,50	11.59	32 (68%)
8	BCL	9	101	-	58,74,74	1.20	4 (6%)	69,115,115	1.53	12 (17%)
10	PC1	H	303	-	19,19,53	2.14	6 (31%)	21,25,61	1.03	1 (4%)
13	SPO	3	102	-	40,41,41	3.52	23 (57%)	47,50,50	10.25	28 (59%)
8	BCL	3	101	-	58,74,74	1.26	5 (8%)	69,115,115	1.42	10 (14%)
8	BCL	1	101	-	48,64,74	1.38	5 (10%)	57,103,115	1.58	13 (22%)
13	SPO	P	101	-	40,41,41	3.65	23 (57%)	47,50,50	10.39	29 (61%)
13	SPO	V	101	-	40,41,41	3.32	21 (52%)	47,50,50	12.23	32 (68%)
13	SPO	J	101	-	40,41,41	3.33	19 (47%)	47,50,50	10.62	34 (72%)
13	SPO	J	103	-	40,41,41	3.59	21 (52%)	47,50,50	10.79	30 (63%)
10	PC1	A	102	-	44,44,53	1.34	6 (13%)	50,52,61	1.14	3 (6%)
13	SPO	E	102	-	40,41,41	3.64	20 (50%)	47,50,50	10.47	32 (68%)
8	BCL	N	101	-	58,74,74	1.26	4 (6%)	69,115,115	1.56	16 (23%)
8	BCL	8	101	-	53,69,74	1.28	3 (5%)	63,109,115	1.41	11 (17%)
10	PC1	H	301	-	39,39,53	1.39	6 (15%)	45,47,61	1.09	2 (4%)
13	SPO	D	103	-	40,41,41	3.55	21 (52%)	47,50,50	10.76	32 (68%)
13	SPO	N	102	-	40,41,41	3.48	22 (55%)	47,50,50	10.55	32 (68%)
13	SPO	T	102	-	40,41,41	3.57	21 (52%)	47,50,50	10.06	31 (65%)
13	SPO	8	102	-	40,41,41	3.57	21 (52%)	47,50,50	11.36	34 (72%)
8	BCL	F	101	-	58,74,74	1.22	4 (6%)	69,115,115	1.44	11 (15%)
14	CDL	H	304	-	77,77,99	1.27	6 (7%)	83,89,111	1.45	6 (7%)
13	SPO	O	104	-	40,41,41	3.41	21 (52%)	47,50,50	9.99	29 (61%)
13	SPO	F	102	-	40,41,41	3.47	21 (52%)	47,50,50	10.27	28 (59%)
8	BCL	1	102	-	53,69,74	1.27	3 (5%)	63,109,115	1.36	9 (14%)
8	BCL	0	102	-	53,69,74	1.24	3 (5%)	63,109,115	1.59	14 (22%)
9	BPB	M	403	-	39,60,70	1.66	2 (5%)	35,89,101	1.42	6 (17%)
8	BCL	D	101	-	58,74,74	1.22	4 (6%)	69,115,115	1.42	10 (14%)
13	SPO	B	101	-	40,41,41	3.37	21 (52%)	47,50,50	10.35	31 (65%)
8	BCL	A	103	-	58,74,74	1.20	3 (5%)	69,115,115	1.45	13 (18%)
8	BCL	K	101	-	58,74,74	1.19	4 (6%)	69,115,115	1.40	11 (15%)
13	SPO	U	104	-	40,41,41	3.48	21 (52%)	47,50,50	10.14	33 (70%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BCL	C	101	-	58,74,74	1.19	3 (5%)	69,115,115	1.48	13 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	3	103	-	-	4/37/137/137	-
13	SPO	U	102	-	-	17/47/47/47	-
13	SPO	X	101	-	-	16/44/44/47	-
8	BCL	R	101	-	-	5/37/137/137	-
10	PC1	H	302	-	-	14/45/45/57	-
13	SPO	O	102	-	-	16/47/47/47	-
11	U10	Y	501	-	-	10/33/57/87	0/1/1/1
13	SPO	M	405	-	-	14/47/47/47	-
8	BCL	L	307	-	-	5/37/137/137	-
13	SPO	I	102	-	-	16/47/47/47	-
8	BCL	L	302	-	-	2/34/134/137	-
14	CDL	M	406	-	-	53/110/110/110	-
8	BCL	M	402	-	-	2/37/137/137	-
13	SPO	3	104	-	-	19/47/47/47	-
10	PC1	D	104	-	-	13/40/40/57	-
8	BCL	L	301	-	-	1/37/137/137	-
13	SPO	D	102	-	-	7/47/47/47	-
10	PC1	L	306	-	-	13/39/39/57	-
8	BCL	S	101	-	-	4/37/137/137	-
8	BCL	E	101	-	-	6/37/137/137	-
11	U10	M	404	-	-	7/45/69/87	0/1/1/1
8	BCL	A	101	-	-	0/37/137/137	-
13	SPO	T	101	-	-	7/47/47/47	-
8	BCL	O	101	-	-	5/37/137/137	-
8	BCL	S	102	-	-	7/37/137/137	-
8	BCL	W	102	-	-	2/37/137/137	-
10	PC1	L	304	-	-	12/38/38/57	-
8	BCL	J	102	-	-	6/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	I	101	-	-	0/37/137/137	-
8	BCL	F	103	-	-	5/37/137/137	-
11	U10	L	308	-	-	6/33/57/87	0/1/1/1
8	BCL	O	103	-	-	7/37/137/137	-
13	SPO	W	103	-	-	20/47/47/47	-
11	U10	L	305	-	-	16/39/63/87	0/1/1/1
8	BCL	7	101	-	-	10/37/137/137	-
13	SPO	0	101	-	-	14/47/47/47	-
13	SPO	9	102	-	-	19/47/47/47	-
8	BCL	U	101	-	-	4/37/137/137	-
8	BCL	Q	101	-	-	0/37/137/137	-
8	BCL	U	103	-	-	11/37/137/137	-
10	PC1	A	104	-	-	15/35/35/57	-
10	PC1	W	101	-	-	12/40/40/57	-
9	BPB	L	303	-	-	6/34/102/105	0/5/6/6
13	SPO	G	101	-	-	15/47/47/47	-
8	BCL	9	101	-	-	5/37/137/137	-
10	PC1	H	303	-	-	6/21/21/57	-
13	SPO	3	102	-	-	7/47/47/47	-
8	BCL	3	101	-	-	0/37/137/137	-
8	BCL	1	101	-	-	3/25/125/137	-
13	SPO	P	101	-	-	13/47/47/47	-
13	SPO	V	101	-	-	14/47/47/47	-
13	SPO	J	101	-	-	16/47/47/47	-
13	SPO	J	103	-	-	18/47/47/47	-
10	PC1	A	102	-	-	17/48/48/57	-
13	SPO	E	102	-	-	13/47/47/47	-
8	BCL	N	101	-	-	10/37/137/137	-
8	BCL	8	101	-	-	3/31/131/137	-
10	PC1	H	301	-	-	15/43/43/57	-
13	SPO	D	103	-	-	13/47/47/47	-
13	SPO	N	102	-	-	22/47/47/47	-
13	SPO	T	102	-	-	18/47/47/47	-
13	SPO	8	102	-	-	23/47/47/47	-
8	BCL	F	101	-	-	4/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	H	304	-	-	37/88/88/110	-
13	SPO	O	104	-	-	16/47/47/47	-
13	SPO	F	102	-	-	12/47/47/47	-
8	BCL	1	102	-	-	6/31/131/137	-
8	BCL	0	102	-	-	4/31/131/137	-
9	BPB	M	403	-	-	6/25/93/105	0/5/6/6
8	BCL	D	101	-	-	0/37/137/137	-
13	SPO	B	101	-	-	13/47/47/47	-
8	BCL	A	103	-	-	4/37/137/137	-
8	BCL	K	101	-	-	0/37/137/137	-
13	SPO	U	104	-	-	20/47/47/47	-
8	BCL	C	101	-	-	9/37/137/137	-

All (789) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	102	SPO	C25-C23	9.18	1.65	1.45
13	T	102	SPO	C16-C17	9.06	1.65	1.45
13	3	104	SPO	C16-C17	8.99	1.65	1.45
9	L	303	BPB	CAC-C3C	8.97	1.56	1.33
13	J	103	SPO	C25-C23	8.88	1.65	1.45
13	3	104	SPO	C25-C23	8.88	1.65	1.45
13	D	103	SPO	C16-C17	8.80	1.64	1.45
13	G	101	SPO	C16-C17	8.79	1.64	1.45
13	D	103	SPO	C25-C23	8.79	1.64	1.45
13	M	405	SPO	C25-C23	8.75	1.64	1.45
13	0	101	SPO	C16-C17	8.66	1.64	1.45
13	U	104	SPO	C25-C23	8.65	1.64	1.45
9	M	403	BPB	CAC-C3C	8.58	1.55	1.33
13	O	102	SPO	C25-C23	8.48	1.64	1.45
13	W	103	SPO	C25-C23	8.39	1.64	1.45
13	P	101	SPO	C16-C17	8.30	1.63	1.45
13	T	102	SPO	C25-C23	8.28	1.63	1.45
13	3	102	SPO	C25-C23	8.24	1.63	1.45
13	P	101	SPO	C25-C23	8.23	1.63	1.45
13	0	101	SPO	C25-C23	8.12	1.63	1.45
13	W	103	SPO	C16-C17	8.11	1.63	1.45
13	J	103	SPO	C16-C17	8.08	1.63	1.45
13	U	102	SPO	C25-C23	8.04	1.63	1.45
13	N	102	SPO	C25-C23	8.03	1.63	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	102	SPO	C16-C17	7.95	1.63	1.45
13	N	102	SPO	C16-C17	7.95	1.63	1.45
13	I	102	SPO	C25-C23	7.90	1.62	1.45
13	9	102	SPO	C16-C17	7.90	1.62	1.45
13	E	102	SPO	C16-C17	7.89	1.62	1.45
13	F	102	SPO	C25-C23	7.88	1.62	1.45
13	8	102	SPO	C16-C17	7.84	1.62	1.45
13	D	102	SPO	C25-C23	7.81	1.62	1.45
13	J	101	SPO	C16-C17	7.80	1.62	1.45
13	T	101	SPO	C16-C17	7.77	1.62	1.45
13	U	104	SPO	C16-C17	7.66	1.62	1.45
13	X	101	SPO	C16-C17	7.66	1.62	1.45
13	V	101	SPO	C16-C17	7.65	1.62	1.45
13	D	102	SPO	C16-C17	7.64	1.62	1.45
13	B	101	SPO	C25-C23	7.61	1.62	1.45
13	B	101	SPO	C16-C17	7.61	1.62	1.45
13	O	104	SPO	C25-C23	7.60	1.62	1.45
13	G	101	SPO	C25-C23	7.60	1.62	1.45
13	I	102	SPO	C16-C17	7.59	1.62	1.45
13	O	104	SPO	C16-C17	7.59	1.62	1.45
13	3	102	SPO	C16-C17	7.57	1.62	1.45
13	J	101	SPO	C25-C23	7.57	1.62	1.45
13	9	102	SPO	C25-C23	7.57	1.62	1.45
13	M	405	SPO	C16-C17	7.55	1.62	1.45
13	D	103	SPO	C11-C12	7.54	1.62	1.45
13	X	101	SPO	C25-C23	7.46	1.62	1.45
13	U	102	SPO	C16-C17	7.41	1.61	1.45
13	O	102	SPO	C16-C17	7.41	1.61	1.45
13	8	102	SPO	C25-C23	7.40	1.61	1.45
13	T	101	SPO	C25-C23	7.24	1.61	1.45
13	V	101	SPO	C25-C23	7.09	1.61	1.45
13	O	102	SPO	C35-C33	6.94	1.65	1.51
13	P	101	SPO	C35-C33	6.87	1.65	1.51
13	9	102	SPO	C35-C33	6.52	1.64	1.51
13	G	101	SPO	C35-C33	6.43	1.64	1.51
13	J	101	SPO	C35-C33	6.33	1.64	1.51
13	3	104	SPO	C11-C12	6.33	1.59	1.45
13	P	101	SPO	C11-C12	6.28	1.59	1.45
13	3	102	SPO	C11-C12	6.27	1.59	1.45
13	I	102	SPO	C35-C33	6.26	1.64	1.51
13	B	101	SPO	C11-C12	6.22	1.59	1.45
13	O	104	SPO	C11-C12	6.21	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	405	SPO	C11-C12	6.20	1.59	1.45
13	T	101	SPO	C11-C12	6.19	1.59	1.45
13	D	102	SPO	C11-C12	6.18	1.59	1.45
11	L	305	U10	C13-C14	6.15	1.47	1.33
13	9	102	SPO	C11-C12	6.10	1.59	1.45
13	T	102	SPO	C11-C12	6.10	1.59	1.45
13	W	103	SPO	C35-C33	6.10	1.64	1.51
13	O	104	SPO	C35-C33	6.09	1.63	1.51
13	U	104	SPO	C11-C12	6.07	1.59	1.45
13	F	102	SPO	C11-C12	6.05	1.58	1.45
13	I	102	SPO	C11-C12	6.05	1.58	1.45
11	M	404	U10	C33-C34	6.03	1.47	1.33
11	L	308	U10	C13-C14	6.01	1.47	1.33
13	J	101	SPO	C11-C12	6.01	1.58	1.45
13	8	102	SPO	C11-C12	6.01	1.58	1.45
13	X	101	SPO	C11-C12	5.99	1.58	1.45
11	Y	501	U10	C23-C24	5.99	1.47	1.33
13	W	103	SPO	C11-C12	5.99	1.58	1.45
11	L	305	U10	C28-C29	5.99	1.47	1.33
11	Y	501	U10	C13-C14	5.99	1.47	1.33
11	L	305	U10	C18-C19	5.98	1.47	1.33
11	L	305	U10	C23-C24	5.97	1.47	1.33
13	V	101	SPO	C11-C12	5.97	1.58	1.45
11	Y	501	U10	C8-C9	5.96	1.47	1.33
13	E	102	SPO	C20-C19	5.95	1.61	1.43
11	M	404	U10	C8-C9	5.95	1.47	1.33
11	Y	501	U10	C18-C19	5.94	1.47	1.33
11	M	404	U10	C18-C19	5.94	1.47	1.33
11	M	404	U10	C28-C29	5.92	1.47	1.33
13	G	101	SPO	C6-C7	5.91	1.58	1.45
13	G	101	SPO	C11-C12	5.91	1.58	1.45
13	E	102	SPO	C30-C28	5.91	1.63	1.51
11	L	308	U10	C8-C9	5.90	1.47	1.33
13	3	104	SPO	C35-C33	5.89	1.63	1.51
13	3	102	SPO	C35-C33	5.89	1.63	1.51
11	M	404	U10	C13-C14	5.88	1.47	1.33
13	8	102	SPO	C30-C28	5.88	1.63	1.51
13	8	102	SPO	C20-C19	5.87	1.61	1.43
11	M	404	U10	C23-C24	5.86	1.47	1.33
11	L	308	U10	C23-C24	5.86	1.47	1.33
11	L	308	U10	C18-C19	5.86	1.47	1.33
13	E	102	SPO	C11-C12	5.84	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V	101	SPO	C35-C33	5.83	1.63	1.51
13	0	101	SPO	C35-C33	5.82	1.63	1.51
11	L	305	U10	C8-C9	5.82	1.46	1.33
13	U	104	SPO	C35-C33	5.80	1.63	1.51
13	J	103	SPO	C35-C33	5.79	1.63	1.51
13	0	101	SPO	C6-C7	5.78	1.58	1.45
13	3	102	SPO	C30-C28	5.73	1.63	1.51
13	J	103	SPO	C6-C7	5.73	1.58	1.45
13	O	102	SPO	C11-C12	5.72	1.58	1.45
13	I	102	SPO	C30-C28	5.72	1.63	1.51
13	P	101	SPO	C20-C19	5.71	1.61	1.43
13	N	102	SPO	C11-C12	5.68	1.58	1.45
13	8	102	SPO	C6-C7	5.67	1.58	1.45
13	3	104	SPO	C30-C28	5.64	1.63	1.51
10	H	303	PC1	O21-C2	-5.64	1.40	1.46
13	D	102	SPO	C35-C33	5.63	1.63	1.51
13	8	102	SPO	C26-C27	5.63	1.60	1.43
13	U	102	SPO	C11-C12	5.62	1.58	1.45
13	F	102	SPO	C30-C28	5.57	1.62	1.51
13	T	102	SPO	C30-C28	5.56	1.62	1.51
13	F	102	SPO	C35-C33	5.55	1.62	1.51
13	P	101	SPO	C30-C28	5.55	1.62	1.51
13	T	101	SPO	C35-C33	5.54	1.62	1.51
13	U	104	SPO	C30-C28	5.54	1.62	1.51
13	G	101	SPO	C30-C28	5.53	1.62	1.51
13	8	102	SPO	C27-C28	5.52	1.39	1.34
13	W	103	SPO	C20-C19	5.52	1.60	1.43
13	0	101	SPO	C11-C12	5.50	1.57	1.45
11	L	308	U10	O3-C3	-5.50	1.23	1.36
11	L	305	U10	O4-C4	-5.49	1.23	1.36
13	P	101	SPO	C6-C7	5.49	1.57	1.45
13	U	102	SPO	C35-C33	5.48	1.62	1.51
13	U	102	SPO	C30-C28	5.48	1.62	1.51
13	U	102	SPO	C6-C7	5.47	1.57	1.45
13	T	102	SPO	C35-C33	5.46	1.62	1.51
13	U	104	SPO	C20-C19	5.46	1.60	1.43
11	Y	501	U10	O3-C3	-5.46	1.23	1.36
11	Y	501	U10	O4-C4	-5.46	1.23	1.36
13	E	102	SPO	C6-C7	5.45	1.57	1.45
13	M	405	SPO	C6-C7	5.44	1.57	1.45
13	W	103	SPO	C6-C7	5.44	1.57	1.45
13	E	102	SPO	C35-C33	5.43	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	102	SPO	C20-C19	5.43	1.60	1.43
13	E	102	SPO	C15-C14	5.43	1.60	1.43
13	F	102	SPO	C6-C7	5.43	1.57	1.45
13	3	104	SPO	C20-C19	5.43	1.60	1.43
13	0	101	SPO	C20-C19	5.42	1.60	1.43
13	9	102	SPO	C20-C19	5.41	1.60	1.43
13	B	101	SPO	C20-C19	5.40	1.60	1.43
13	T	101	SPO	C30-C28	5.40	1.62	1.51
13	T	101	SPO	C6-C7	5.40	1.57	1.45
13	N	102	SPO	C30-C28	5.39	1.62	1.51
11	M	404	U10	O4-C4	-5.39	1.23	1.36
13	J	103	SPO	C11-C12	5.39	1.57	1.45
13	3	104	SPO	C26-C27	5.39	1.60	1.43
11	L	308	U10	O4-C4	-5.38	1.23	1.36
13	D	103	SPO	C20-C19	5.38	1.60	1.43
13	I	102	SPO	C6-C7	5.38	1.57	1.45
13	3	104	SPO	C15-C14	5.38	1.60	1.43
13	B	101	SPO	C6-C7	5.37	1.57	1.45
13	D	103	SPO	C6-C7	5.37	1.57	1.45
13	V	101	SPO	C6-C7	5.36	1.57	1.45
13	O	104	SPO	C20-C19	5.36	1.60	1.43
13	9	102	SPO	C6-C7	5.35	1.57	1.45
11	M	404	U10	O3-C3	-5.35	1.23	1.36
11	L	305	U10	O3-C3	-5.34	1.23	1.36
13	B	101	SPO	C35-C33	5.33	1.62	1.51
13	I	102	SPO	C20-C19	5.33	1.60	1.43
13	X	101	SPO	C6-C7	5.32	1.57	1.45
13	N	102	SPO	C6-C7	5.32	1.57	1.45
11	M	404	U10	C38-C39	5.31	1.47	1.32
13	M	405	SPO	C35-C33	5.30	1.62	1.51
13	D	102	SPO	C6-C7	5.30	1.57	1.45
13	T	102	SPO	C20-C19	5.30	1.59	1.43
13	3	102	SPO	C6-C7	5.30	1.57	1.45
13	O	104	SPO	C30-C28	5.29	1.62	1.51
13	X	101	SPO	C35-C33	5.28	1.62	1.51
13	T	102	SPO	C6-C7	5.28	1.57	1.45
13	V	101	SPO	C30-C28	5.28	1.62	1.51
13	3	104	SPO	C6-C7	5.27	1.57	1.45
13	J	103	SPO	C15-C14	5.27	1.59	1.43
13	G	101	SPO	C26-C27	5.26	1.59	1.43
13	X	101	SPO	C20-C19	5.26	1.59	1.43
13	N	102	SPO	C35-C33	5.25	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	U	102	SPO	C20-C19	5.25	1.59	1.43
13	J	103	SPO	C20-C19	5.25	1.59	1.43
11	Y	501	U10	C28-C29	5.23	1.47	1.32
13	N	102	SPO	C20-C19	5.23	1.59	1.43
13	O	102	SPO	C6-C7	5.22	1.57	1.45
13	8	102	SPO	C35-C33	5.22	1.62	1.51
13	O	104	SPO	C6-C7	5.22	1.57	1.45
13	3	104	SPO	C27-C28	5.22	1.39	1.34
13	D	103	SPO	C30-C28	5.21	1.62	1.51
11	L	308	U10	C28-C29	5.21	1.47	1.32
13	9	102	SPO	C30-C28	5.20	1.62	1.51
13	3	102	SPO	C20-C19	5.20	1.59	1.43
13	D	102	SPO	C30-C28	5.19	1.62	1.51
13	T	102	SPO	C15-C14	5.18	1.59	1.43
13	T	101	SPO	C20-C19	5.17	1.59	1.43
11	L	305	U10	C33-C34	5.16	1.47	1.32
13	8	102	SPO	C15-C14	5.15	1.59	1.43
13	U	104	SPO	C6-C7	5.15	1.57	1.45
13	0	101	SPO	C30-C28	5.15	1.62	1.51
13	X	101	SPO	C30-C28	5.13	1.62	1.51
13	D	102	SPO	C20-C19	5.13	1.59	1.43
13	G	101	SPO	C20-C19	5.11	1.59	1.43
13	J	101	SPO	C30-C28	5.11	1.61	1.51
13	E	102	SPO	C26-C27	5.11	1.59	1.43
13	B	101	SPO	C30-C28	5.10	1.61	1.51
13	M	405	SPO	C20-C19	5.09	1.59	1.43
13	V	101	SPO	C20-C19	5.08	1.59	1.43
13	O	102	SPO	C20-C19	5.07	1.59	1.43
13	T	102	SPO	C26-C27	5.07	1.59	1.43
13	P	101	SPO	C26-C27	5.04	1.59	1.43
13	W	103	SPO	C15-C14	5.04	1.59	1.43
13	O	102	SPO	C30-C28	5.03	1.61	1.51
13	W	103	SPO	C30-C28	5.01	1.61	1.51
13	J	101	SPO	C26-C27	5.00	1.58	1.43
13	P	101	SPO	C15-C14	5.00	1.58	1.43
13	J	103	SPO	C30-C28	4.99	1.61	1.51
13	F	102	SPO	C26-C27	4.98	1.58	1.43
13	J	103	SPO	C26-C27	4.98	1.58	1.43
13	O	104	SPO	C26-C27	4.98	1.58	1.43
13	J	101	SPO	C20-C19	4.97	1.58	1.43
13	N	102	SPO	C15-C14	4.96	1.58	1.43
13	B	101	SPO	C15-C14	4.96	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	103	SPO	C35-C33	4.96	1.61	1.51
13	J	101	SPO	C6-C7	4.95	1.56	1.45
13	X	101	SPO	C26-C27	4.95	1.58	1.43
13	G	101	SPO	C15-C14	4.94	1.58	1.43
8	3	103	BCL	C1B-NB	4.93	1.39	1.35
13	N	102	SPO	C26-C27	4.93	1.58	1.43
13	0	101	SPO	C15-C14	4.93	1.58	1.43
13	0	101	SPO	C26-C27	4.93	1.58	1.43
13	3	104	SPO	C21-C22	4.93	1.58	1.43
8	U	103	BCL	C1B-NB	4.92	1.39	1.35
13	I	102	SPO	C26-C27	4.92	1.58	1.43
8	J	102	BCL	C1B-NB	4.92	1.39	1.35
8	8	101	BCL	C1B-NB	4.91	1.39	1.35
13	O	102	SPO	C26-C27	4.90	1.58	1.43
13	F	102	SPO	C15-C14	4.88	1.58	1.43
13	D	102	SPO	C26-C27	4.88	1.58	1.43
13	9	102	SPO	C26-C27	4.88	1.58	1.43
13	W	103	SPO	C26-C27	4.87	1.58	1.43
13	E	102	SPO	C21-C22	4.87	1.58	1.43
8	1	101	BCL	MG-NA	4.87	2.17	2.06
13	3	102	SPO	C26-C27	4.85	1.58	1.43
13	T	101	SPO	C26-C27	4.84	1.58	1.43
13	M	405	SPO	C26-C27	4.83	1.58	1.43
13	U	104	SPO	C26-C27	4.83	1.58	1.43
8	3	101	BCL	MG-NA	4.82	2.17	2.06
8	S	102	BCL	MG-NA	4.81	2.17	2.06
8	1	102	BCL	C1B-NB	4.81	1.39	1.35
13	V	101	SPO	C15-C14	4.80	1.58	1.43
8	N	101	BCL	C1B-NB	4.80	1.39	1.35
13	X	101	SPO	C15-C14	4.79	1.58	1.43
8	W	102	BCL	C1B-NB	4.79	1.39	1.35
13	B	101	SPO	C26-C27	4.79	1.58	1.43
13	D	103	SPO	C15-C14	4.76	1.58	1.43
8	R	101	BCL	MG-NA	4.76	2.17	2.06
8	A	103	BCL	C1B-NB	4.76	1.39	1.35
8	U	101	BCL	MG-NA	4.75	2.17	2.06
13	V	101	SPO	C26-C27	4.75	1.58	1.43
13	M	405	SPO	C21-C22	4.74	1.58	1.43
8	3	101	BCL	C1B-NB	4.74	1.39	1.35
8	F	101	BCL	MG-NA	4.74	2.17	2.06
13	M	405	SPO	C30-C28	4.73	1.61	1.51
8	O	103	BCL	MG-NA	4.73	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3	103	BCL	MG-NA	4.73	2.17	2.06
8	1	101	BCL	C1B-NB	4.72	1.39	1.35
8	S	101	BCL	C1B-NB	4.72	1.39	1.35
8	D	101	BCL	MG-NA	4.72	2.17	2.06
13	T	101	SPO	C15-C14	4.71	1.58	1.43
13	M	405	SPO	C15-C14	4.71	1.58	1.43
8	L	301	BCL	MG-NA	4.71	2.17	2.06
13	0	101	SPO	C10-C9	4.71	1.58	1.43
8	O	101	BCL	MG-NA	4.70	2.17	2.06
13	U	102	SPO	C26-C27	4.70	1.58	1.43
13	U	104	SPO	C15-C14	4.70	1.58	1.43
8	K	101	BCL	MG-NA	4.70	2.17	2.06
8	1	102	BCL	MG-NA	4.70	2.17	2.06
8	F	103	BCL	C1B-NB	4.70	1.39	1.35
8	O	103	BCL	C1B-NB	4.70	1.39	1.35
8	M	402	BCL	MG-NA	4.70	2.17	2.06
13	D	102	SPO	C15-C14	4.70	1.58	1.43
13	E	102	SPO	C27-C28	4.70	1.39	1.34
8	U	103	BCL	MG-NA	4.70	2.17	2.06
8	R	101	BCL	C1B-NB	4.69	1.39	1.35
13	P	101	SPO	C10-C9	4.69	1.58	1.43
13	U	102	SPO	C15-C14	4.68	1.58	1.43
13	I	102	SPO	C15-C14	4.67	1.57	1.43
8	W	102	BCL	MG-NA	4.67	2.17	2.06
13	J	103	SPO	C21-C22	4.67	1.57	1.43
13	F	102	SPO	C10-C9	4.67	1.57	1.43
8	S	101	BCL	MG-NA	4.66	2.17	2.06
8	7	101	BCL	MG-NA	4.66	2.17	2.06
13	B	101	SPO	C10-C9	4.66	1.57	1.43
13	9	102	SPO	C15-C14	4.65	1.57	1.43
8	9	101	BCL	MG-NA	4.65	2.17	2.06
13	P	101	SPO	C21-C22	4.65	1.57	1.43
13	J	101	SPO	C15-C14	4.64	1.57	1.43
8	A	101	BCL	C1B-NB	4.64	1.39	1.35
8	S	102	BCL	C1B-NB	4.64	1.39	1.35
8	A	101	BCL	MG-NA	4.63	2.17	2.06
8	F	101	BCL	C1B-NB	4.63	1.39	1.35
13	O	104	SPO	C15-C14	4.63	1.57	1.43
8	L	301	BCL	C1B-NB	4.63	1.39	1.35
8	C	101	BCL	C1B-NB	4.62	1.39	1.35
8	I	101	BCL	C1B-NB	4.62	1.39	1.35
8	K	101	BCL	C1B-NB	4.62	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	302	BCL	C1B-NB	4.62	1.39	1.35
8	E	101	BCL	C1B-NB	4.61	1.39	1.35
8	Q	101	BCL	MG-NA	4.61	2.17	2.06
8	J	102	BCL	MG-NA	4.60	2.17	2.06
8	A	103	BCL	MG-NA	4.60	2.17	2.06
8	0	102	BCL	C1B-NB	4.60	1.39	1.35
8	E	101	BCL	MG-NA	4.59	2.17	2.06
8	7	101	BCL	C1B-NB	4.58	1.39	1.35
8	D	101	BCL	C1B-NB	4.58	1.39	1.35
13	O	102	SPO	C15-C14	4.58	1.57	1.43
13	8	102	SPO	C21-C22	4.58	1.57	1.43
8	Q	101	BCL	C1B-NB	4.56	1.39	1.35
8	8	101	BCL	MG-NA	4.56	2.17	2.06
13	T	101	SPO	C10-C9	4.56	1.57	1.43
8	N	101	BCL	MG-NA	4.56	2.17	2.06
8	0	102	BCL	MG-NA	4.56	2.17	2.06
13	9	102	SPO	C10-C9	4.55	1.57	1.43
8	F	103	BCL	MG-NA	4.55	2.17	2.06
13	N	102	SPO	C21-C22	4.54	1.57	1.43
13	E	102	SPO	C10-C9	4.54	1.57	1.43
13	0	101	SPO	C21-C22	4.54	1.57	1.43
13	X	101	SPO	C10-C9	4.53	1.57	1.43
8	U	101	BCL	C1B-NB	4.53	1.39	1.35
8	L	302	BCL	MG-NA	4.53	2.17	2.06
13	U	104	SPO	C21-C22	4.52	1.57	1.43
8	L	307	BCL	C1B-NB	4.52	1.39	1.35
13	D	103	SPO	C26-C27	4.52	1.57	1.43
13	3	102	SPO	C15-C14	4.52	1.57	1.43
13	G	101	SPO	C10-C9	4.52	1.57	1.43
13	T	102	SPO	C10-C9	4.52	1.57	1.43
13	T	102	SPO	C27-C28	4.52	1.38	1.34
8	C	101	BCL	MG-NA	4.51	2.17	2.06
13	J	103	SPO	C10-C9	4.51	1.57	1.43
8	9	101	BCL	C1B-NB	4.50	1.39	1.35
13	W	103	SPO	C10-C9	4.50	1.57	1.43
8	O	101	BCL	C1B-NB	4.49	1.39	1.35
13	3	104	SPO	C10-C9	4.49	1.57	1.43
13	I	102	SPO	C10-C9	4.49	1.57	1.43
13	N	102	SPO	C10-C9	4.47	1.57	1.43
10	H	303	PC1	O21-C21	4.46	1.43	1.33
13	D	102	SPO	C10-C9	4.46	1.57	1.43
13	8	102	SPO	C10-C9	4.46	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	102	SPO	C10-C9	4.45	1.57	1.43
8	L	307	BCL	MG-NA	4.44	2.16	2.06
13	F	102	SPO	C21-C22	4.43	1.57	1.43
13	O	102	SPO	C10-C9	4.43	1.57	1.43
13	U	104	SPO	C10-C9	4.43	1.57	1.43
13	W	103	SPO	C21-C22	4.43	1.57	1.43
13	U	102	SPO	C21-C22	4.43	1.57	1.43
8	I	101	BCL	MG-NA	4.40	2.16	2.06
13	9	102	SPO	C21-C22	4.37	1.57	1.43
13	M	405	SPO	C10-C9	4.35	1.56	1.43
13	O	104	SPO	C21-C22	4.34	1.56	1.43
13	D	103	SPO	C21-C22	4.33	1.56	1.43
13	3	102	SPO	C27-C28	4.33	1.38	1.34
13	G	101	SPO	C21-C22	4.32	1.56	1.43
13	U	102	SPO	C10-C9	4.31	1.56	1.43
13	O	102	SPO	C21-C22	4.30	1.56	1.43
13	O	104	SPO	C10-C9	4.30	1.56	1.43
13	I	102	SPO	C21-C22	4.30	1.56	1.43
13	V	101	SPO	C21-C22	4.28	1.56	1.43
13	V	101	SPO	C10-C9	4.28	1.56	1.43
8	M	402	BCL	C1B-NB	4.27	1.39	1.35
13	P	101	SPO	C27-C28	4.27	1.38	1.34
13	J	103	SPO	C14-C12	4.27	1.41	1.35
13	G	101	SPO	C4-C5	4.26	1.56	1.50
13	3	102	SPO	C21-C22	4.25	1.56	1.43
13	D	103	SPO	C10-C9	4.25	1.56	1.43
13	D	102	SPO	C21-C22	4.25	1.56	1.43
13	T	101	SPO	C21-C22	4.24	1.56	1.43
13	I	102	SPO	C27-C28	4.22	1.38	1.34
13	X	101	SPO	C21-C22	4.20	1.56	1.43
13	J	101	SPO	C21-C22	4.17	1.56	1.43
13	J	101	SPO	C10-C9	4.16	1.56	1.43
13	B	101	SPO	C21-C22	4.15	1.56	1.43
13	J	103	SPO	C4-C5	4.11	1.56	1.50
13	O	104	SPO	C27-C28	4.08	1.38	1.34
13	T	102	SPO	C21-C22	4.07	1.56	1.43
13	F	102	SPO	C4-C5	4.05	1.56	1.50
13	J	103	SPO	C27-C28	4.03	1.38	1.34
13	F	102	SPO	C27-C28	4.00	1.38	1.34
13	O	102	SPO	C27-C28	3.97	1.38	1.34
13	J	101	SPO	C27-C28	3.90	1.38	1.34
13	N	102	SPO	C27-C28	3.89	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	104	SPO	C4-C5	3.89	1.56	1.50
13	D	102	SPO	C4-C5	3.87	1.56	1.50
10	A	102	PC1	O31-C31	3.85	1.44	1.33
13	U	102	SPO	C27-C28	3.84	1.38	1.34
13	V	101	SPO	C4-C5	3.82	1.56	1.50
13	X	101	SPO	C4-C5	3.79	1.56	1.50
13	B	101	SPO	C4-C5	3.78	1.56	1.50
13	M	405	SPO	C27-C28	3.78	1.38	1.34
13	3	102	SPO	C4-C5	3.78	1.56	1.50
13	P	101	SPO	C4-C5	3.77	1.56	1.50
13	0	101	SPO	C27-C28	3.76	1.38	1.34
13	I	102	SPO	C4-C5	3.72	1.56	1.50
10	W	101	PC1	O31-C31	3.71	1.44	1.33
9	L	303	BPB	CBD-CGD	-3.71	1.47	1.52
13	E	102	SPO	C14-C12	3.71	1.40	1.35
13	9	102	SPO	C4-C5	3.70	1.56	1.50
13	U	104	SPO	C4-C5	3.69	1.56	1.50
13	W	103	SPO	C27-C28	3.69	1.38	1.34
10	A	104	PC1	O31-C31	3.69	1.44	1.33
13	O	102	SPO	C4-C5	3.69	1.56	1.50
10	L	306	PC1	O31-C31	3.68	1.44	1.33
13	0	101	SPO	C4-C5	3.66	1.56	1.50
13	D	102	SPO	C27-C28	3.65	1.37	1.34
9	M	403	BPB	CBD-CGD	-3.65	1.47	1.52
13	8	102	SPO	C4-C5	3.64	1.55	1.50
10	H	301	PC1	O31-C31	3.64	1.44	1.33
13	T	101	SPO	C4-C5	3.63	1.55	1.50
13	3	104	SPO	C31-C32	3.63	1.62	1.50
13	N	102	SPO	C4-C5	3.62	1.55	1.50
10	H	302	PC1	O31-C31	3.62	1.43	1.33
13	D	103	SPO	C4-C5	3.59	1.55	1.50
13	U	104	SPO	C27-C28	3.59	1.37	1.34
10	D	104	PC1	O31-C31	3.58	1.43	1.33
10	L	304	PC1	O31-C31	3.57	1.43	1.33
13	E	102	SPO	C4-C5	3.57	1.55	1.50
13	G	101	SPO	C27-C28	3.57	1.37	1.34
13	T	102	SPO	C4-C5	3.56	1.55	1.50
13	T	101	SPO	C27-C28	3.56	1.37	1.34
13	N	102	SPO	C13-C12	3.51	1.58	1.50
13	M	405	SPO	C4-C5	3.51	1.55	1.50
13	B	101	SPO	C27-C28	3.49	1.37	1.34
13	3	104	SPO	C32-C33	3.45	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	103	SPO	C4-C5	3.43	1.55	1.50
13	9	102	SPO	C27-C28	3.42	1.37	1.34
13	3	102	SPO	C31-C32	3.40	1.61	1.50
13	P	101	SPO	C31-C32	3.39	1.61	1.50
13	D	103	SPO	C27-C28	3.38	1.37	1.34
11	L	305	U10	C4-C5	-3.38	1.39	1.48
13	D	103	SPO	C18-C17	3.37	1.57	1.50
11	Y	501	U10	C4-C5	-3.37	1.39	1.48
13	G	101	SPO	C31-C32	3.36	1.61	1.50
8	U	103	BCL	MG-NC	3.36	2.14	2.06
8	R	101	BCL	MG-NC	3.32	2.14	2.06
13	O	104	SPO	C4-C5	3.32	1.55	1.50
14	H	304	CDL	OA6-CA5	3.32	1.43	1.34
13	X	101	SPO	C27-C28	3.32	1.37	1.34
8	O	103	BCL	MG-NC	3.31	2.14	2.06
8	3	101	BCL	MG-NC	3.30	2.14	2.06
11	L	308	U10	C4-C5	-3.30	1.39	1.48
8	3	103	BCL	MG-NC	3.30	2.14	2.06
11	L	308	U10	C3-C2	-3.28	1.39	1.48
8	D	101	BCL	MG-NC	3.27	2.14	2.06
8	1	102	BCL	MG-NC	3.27	2.14	2.06
8	S	102	BCL	MG-NC	3.26	2.14	2.06
11	M	404	U10	C4-C5	-3.25	1.39	1.48
11	Y	501	U10	C3-C2	-3.25	1.39	1.48
13	J	103	SPO	C32-C33	3.25	1.40	1.33
8	L	301	BCL	MG-NC	3.25	2.14	2.06
8	F	101	BCL	MG-NC	3.24	2.14	2.06
13	O	102	SPO	C31-C32	3.24	1.61	1.50
8	1	101	BCL	MG-NC	3.23	2.14	2.06
13	3	102	SPO	C13-C12	3.23	1.57	1.50
13	3	102	SPO	C32-C33	3.23	1.40	1.33
14	M	406	CDL	OA6-CA5	3.23	1.43	1.34
8	W	102	BCL	MG-NC	3.22	2.13	2.06
8	J	102	BCL	MG-NC	3.22	2.13	2.06
13	M	405	SPO	C13-C12	3.19	1.57	1.50
8	N	101	BCL	MG-NC	3.19	2.13	2.06
8	E	101	BCL	MG-NC	3.19	2.13	2.06
10	L	306	PC1	O21-C21	3.19	1.43	1.34
13	T	101	SPO	C13-C12	3.18	1.57	1.50
11	M	404	U10	C3-C2	-3.18	1.39	1.48
8	A	101	BCL	MG-NC	3.18	2.13	2.06
8	Q	101	BCL	MG-NC	3.18	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	307	BCL	MG-NC	3.17	2.13	2.06
8	7	101	BCL	MG-NC	3.16	2.13	2.06
14	H	304	CDL	OB8-CB7	3.16	1.42	1.33
8	9	101	BCL	MG-NC	3.15	2.13	2.06
13	J	103	SPO	C31-C32	3.15	1.60	1.50
8	I	101	BCL	O1A-CGA	-3.14	1.13	1.22
13	0	101	SPO	C18-C17	3.14	1.57	1.50
8	O	101	BCL	MG-NC	3.12	2.13	2.06
8	U	101	BCL	MG-NC	3.12	2.13	2.06
13	O	104	SPO	C13-C12	3.11	1.57	1.50
14	H	304	CDL	OA8-CA7	3.11	1.42	1.33
13	3	104	SPO	C14-C12	3.11	1.39	1.35
8	K	101	BCL	MG-NC	3.10	2.13	2.06
14	M	406	CDL	OA8-CA7	3.09	1.42	1.33
11	L	305	U10	C3-C2	-3.08	1.40	1.48
10	A	104	PC1	O21-C21	3.08	1.43	1.34
14	M	406	CDL	OB6-CB5	3.07	1.43	1.34
10	W	101	PC1	O21-C21	3.07	1.43	1.34
14	M	406	CDL	OB8-CB7	3.07	1.42	1.33
8	8	101	BCL	MG-NC	3.06	2.13	2.06
13	T	102	SPO	C13-C12	3.06	1.57	1.50
13	J	101	SPO	C13-C12	3.06	1.57	1.50
13	G	101	SPO	C18-C17	3.06	1.57	1.50
13	U	104	SPO	C32-C33	3.05	1.40	1.33
13	I	102	SPO	C31-C32	3.05	1.60	1.50
13	D	102	SPO	C13-C12	3.05	1.57	1.50
13	X	101	SPO	C13-C12	3.05	1.57	1.50
13	U	102	SPO	C4-C5	3.05	1.55	1.50
8	S	101	BCL	MG-NC	3.05	2.13	2.06
13	3	102	SPO	C18-C17	3.04	1.57	1.50
8	A	103	BCL	MG-NC	3.04	2.13	2.06
13	F	102	SPO	C31-C32	3.04	1.60	1.50
13	3	104	SPO	C13-C12	3.04	1.57	1.50
13	U	104	SPO	C31-C32	3.04	1.60	1.50
8	0	102	BCL	MG-NC	3.04	2.13	2.06
13	U	104	SPO	C13-C12	3.04	1.57	1.50
8	F	103	BCL	MG-NC	3.04	2.13	2.06
8	C	101	BCL	MG-NC	3.04	2.13	2.06
13	W	103	SPO	C31-C32	3.02	1.60	1.50
10	A	102	PC1	O21-C21	3.02	1.42	1.34
13	P	101	SPO	C32-C33	3.01	1.40	1.33
13	V	101	SPO	C13-C12	3.01	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	101	SPO	C31-C32	3.00	1.60	1.50
8	I	101	BCL	MG-NC	3.00	2.13	2.06
13	8	102	SPO	C31-C32	2.99	1.60	1.50
13	D	103	SPO	C13-C12	2.99	1.57	1.50
14	H	304	CDL	OB6-CB5	2.97	1.42	1.34
10	D	104	PC1	O21-C21	2.97	1.42	1.34
13	D	102	SPO	C18-C17	2.97	1.57	1.50
13	9	102	SPO	C31-C32	2.96	1.60	1.50
13	9	102	SPO	C13-C12	2.96	1.57	1.50
13	0	101	SPO	C13-C12	2.96	1.57	1.50
10	L	304	PC1	O21-C21	2.95	1.42	1.34
8	L	302	BCL	MG-NC	2.95	2.13	2.06
13	D	102	SPO	C31-C32	2.95	1.60	1.50
13	V	101	SPO	C18-C17	2.95	1.57	1.50
13	G	101	SPO	C13-C12	2.94	1.57	1.50
13	I	102	SPO	C13-C12	2.93	1.56	1.50
13	O	102	SPO	C18-C17	2.93	1.56	1.50
13	N	102	SPO	C18-C17	2.92	1.56	1.50
13	F	102	SPO	C18-C17	2.92	1.56	1.50
8	L	301	BCL	O1A-CGA	-2.92	1.13	1.22
13	O	104	SPO	C18-C17	2.91	1.56	1.50
13	J	101	SPO	C18-C17	2.91	1.56	1.50
8	M	402	BCL	MG-NC	2.89	2.13	2.06
13	G	101	SPO	C14-C12	2.89	1.39	1.35
10	H	303	PC1	O31-C31	2.89	1.44	1.33
13	W	103	SPO	C13-C12	2.89	1.56	1.50
13	V	101	SPO	C27-C28	2.89	1.37	1.34
13	8	102	SPO	C14-C12	2.88	1.39	1.35
13	8	102	SPO	C13-C12	2.88	1.56	1.50
11	L	305	U10	C6-C5	-2.87	1.38	1.46
13	O	102	SPO	C13-C12	2.86	1.56	1.50
13	V	101	SPO	C30-C31	2.86	1.63	1.53
13	I	102	SPO	C18-C17	2.86	1.56	1.50
13	9	102	SPO	C18-C17	2.86	1.56	1.50
13	T	101	SPO	C31-C32	2.86	1.59	1.50
13	N	102	SPO	C8-C7	2.86	1.56	1.50
13	T	102	SPO	C31-C32	2.85	1.59	1.50
13	T	102	SPO	C32-C33	2.85	1.39	1.33
13	U	102	SPO	C13-C12	2.84	1.56	1.50
13	I	102	SPO	C32-C33	2.84	1.39	1.33
10	H	302	PC1	O21-C21	2.83	1.42	1.34
13	B	101	SPO	C13-C12	2.83	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	104	SPO	C30-C31	2.83	1.63	1.53
13	P	101	SPO	C13-C12	2.83	1.56	1.50
13	P	101	SPO	C30-C31	2.83	1.63	1.53
13	T	101	SPO	C18-C17	2.82	1.56	1.50
13	X	101	SPO	C31-C32	2.82	1.59	1.50
13	N	102	SPO	C32-C33	2.82	1.39	1.33
13	V	101	SPO	C31-C32	2.82	1.59	1.50
13	0	101	SPO	C31-C32	2.81	1.59	1.50
13	U	104	SPO	C18-C17	2.81	1.56	1.50
13	U	102	SPO	C18-C17	2.81	1.56	1.50
13	J	101	SPO	C4-C5	2.80	1.54	1.50
13	8	102	SPO	C32-C33	2.80	1.39	1.33
13	F	102	SPO	C13-C12	2.80	1.56	1.50
13	W	103	SPO	C18-C17	2.80	1.56	1.50
13	8	102	SPO	C30-C31	2.79	1.63	1.53
13	O	104	SPO	C32-C33	2.79	1.39	1.33
13	D	102	SPO	C32-C33	2.78	1.39	1.33
13	O	104	SPO	C31-C32	2.78	1.59	1.50
13	E	102	SPO	C30-C31	2.78	1.63	1.53
13	E	102	SPO	C31-C32	2.78	1.59	1.50
13	8	102	SPO	C18-C17	2.77	1.56	1.50
13	B	101	SPO	C18-C17	2.76	1.56	1.50
13	T	101	SPO	C32-C33	2.75	1.39	1.33
13	P	101	SPO	C18-C17	2.75	1.56	1.50
13	N	102	SPO	C14-C12	2.74	1.39	1.35
13	E	102	SPO	C32-C33	2.74	1.39	1.33
13	D	103	SPO	C31-C32	2.74	1.59	1.50
8	9	101	BCL	O1A-CGA	-2.74	1.14	1.22
10	H	301	PC1	O21-C2	-2.74	1.39	1.46
10	H	301	PC1	O21-C21	2.73	1.42	1.34
13	U	102	SPO	C31-C32	2.73	1.59	1.50
13	T	102	SPO	C8-C7	2.73	1.56	1.50
13	D	103	SPO	C8-C7	2.71	1.56	1.50
13	9	102	SPO	C32-C33	2.71	1.39	1.33
13	M	405	SPO	C31-C32	2.69	1.59	1.50
11	L	308	U10	C6-C1	2.68	1.40	1.35
11	L	308	U10	C6-C5	-2.67	1.39	1.46
8	1	101	BCL	O1A-CGA	-2.67	1.14	1.22
13	E	102	SPO	C13-C12	2.67	1.56	1.50
13	J	103	SPO	C8-C7	2.66	1.56	1.50
8	O	101	BCL	O1A-CGA	-2.66	1.14	1.22
8	Q	101	BCL	O1A-CGA	-2.65	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	404	U10	C6-C5	-2.65	1.39	1.46
13	X	101	SPO	C18-C17	2.65	1.56	1.50
13	T	102	SPO	C30-C31	2.64	1.62	1.53
13	3	102	SPO	C24-C23	2.62	1.56	1.50
13	M	405	SPO	C32-C33	2.62	1.39	1.33
13	W	103	SPO	C32-C33	2.60	1.39	1.33
13	P	101	SPO	C35-C36	2.60	1.62	1.53
13	U	104	SPO	C30-C31	2.60	1.62	1.53
13	3	102	SPO	C30-C31	2.60	1.62	1.53
13	M	405	SPO	C18-C17	2.60	1.56	1.50
13	G	101	SPO	C30-C31	2.60	1.62	1.53
13	F	102	SPO	C32-C33	2.59	1.39	1.33
10	D	104	PC1	O21-C2	-2.59	1.40	1.46
13	3	104	SPO	C24-C23	2.58	1.56	1.50
13	I	102	SPO	C30-C31	2.57	1.62	1.53
8	3	101	BCL	O1A-CGA	-2.57	1.14	1.22
13	X	101	SPO	C32-C33	2.57	1.39	1.33
13	W	103	SPO	C14-C12	2.56	1.39	1.35
13	O	102	SPO	C24-C23	2.56	1.56	1.50
10	H	302	PC1	O21-C2	-2.55	1.40	1.46
13	0	101	SPO	C32-C33	2.54	1.39	1.33
13	U	102	SPO	C32-C33	2.53	1.39	1.33
13	O	104	SPO	C30-C31	2.53	1.62	1.53
13	E	102	SPO	C24-C23	2.52	1.56	1.50
13	N	102	SPO	C31-C32	2.52	1.58	1.50
13	G	101	SPO	C8-C7	2.52	1.56	1.50
13	N	102	SPO	C24-C23	2.52	1.56	1.50
8	S	101	BCL	O1A-CGA	-2.52	1.15	1.22
13	N	102	SPO	C30-C31	2.51	1.62	1.53
10	A	104	PC1	O21-C2	-2.50	1.40	1.46
13	P	101	SPO	C24-C23	2.50	1.56	1.50
13	M	405	SPO	C8-C7	2.50	1.56	1.50
14	H	304	CDL	OB6-CB4	-2.49	1.40	1.46
10	W	101	PC1	O21-C2	-2.49	1.40	1.46
11	M	404	U10	C6-C1	2.49	1.39	1.35
13	D	103	SPO	C32-C33	2.49	1.38	1.33
11	Y	501	U10	C6-C1	2.49	1.39	1.35
11	Y	501	U10	C6-C5	-2.48	1.39	1.46
14	M	406	CDL	OA6-CA4	-2.47	1.40	1.46
13	G	101	SPO	C32-C33	2.47	1.38	1.33
13	U	102	SPO	C8-C7	2.47	1.56	1.50
10	H	301	PC1	P-O13	2.46	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	101	SPO	C31-C32	2.46	1.58	1.50
13	U	104	SPO	C24-C23	2.45	1.55	1.50
10	L	304	PC1	O21-C2	-2.44	1.40	1.46
13	F	102	SPO	C30-C31	2.44	1.61	1.53
13	8	102	SPO	C24-C23	2.44	1.55	1.50
13	D	102	SPO	C30-C31	2.44	1.61	1.53
13	W	103	SPO	C24-C23	2.43	1.55	1.50
13	J	103	SPO	C30-C31	2.43	1.61	1.53
13	B	101	SPO	C32-C33	2.43	1.38	1.33
13	0	101	SPO	C30-C31	2.43	1.61	1.53
13	3	104	SPO	C8-C7	2.43	1.55	1.50
13	J	103	SPO	C24-C23	2.42	1.55	1.50
13	O	104	SPO	C8-C7	2.41	1.55	1.50
13	M	405	SPO	C24-C23	2.41	1.55	1.50
13	J	101	SPO	C8-C7	2.41	1.55	1.50
13	U	102	SPO	C30-C31	2.41	1.61	1.53
8	L	307	BCL	O1A-CGA	-2.40	1.15	1.22
13	F	102	SPO	C8-C7	2.40	1.55	1.50
13	D	102	SPO	C24-C23	2.40	1.55	1.50
13	3	102	SPO	C36-C37	2.40	1.58	1.50
13	O	102	SPO	C30-C31	2.40	1.61	1.53
10	A	102	PC1	O21-C2	-2.39	1.40	1.46
10	A	102	PC1	P-O13	2.39	1.69	1.59
13	T	101	SPO	C8-C7	2.39	1.55	1.50
13	T	101	SPO	C30-C31	2.38	1.61	1.53
13	I	102	SPO	C24-C23	2.37	1.55	1.50
10	A	104	PC1	P-O11	2.37	1.68	1.59
13	M	405	SPO	C14-C12	2.37	1.38	1.35
14	M	406	CDL	OB6-CB4	-2.37	1.40	1.46
13	J	101	SPO	C24-C23	2.36	1.55	1.50
11	M	404	U10	C1-C2	-2.36	1.38	1.47
13	3	102	SPO	C8-C7	2.35	1.55	1.50
10	L	306	PC1	O21-C2	-2.35	1.40	1.46
13	T	102	SPO	C18-C17	2.35	1.55	1.50
10	H	303	PC1	P-O11	2.35	1.68	1.59
13	0	101	SPO	C24-C23	2.35	1.55	1.50
8	F	101	BCL	O1A-CGA	-2.34	1.15	1.22
8	K	101	BCL	O1A-CGA	-2.33	1.15	1.22
13	P	101	SPO	C8-C7	2.33	1.55	1.50
10	W	101	PC1	P-O13	2.33	1.68	1.59
13	J	103	SPO	C13-C12	2.33	1.55	1.50
13	9	102	SPO	C30-C31	2.32	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	102	SPO	C8-C7	2.32	1.55	1.50
13	9	102	SPO	C8-C7	2.32	1.55	1.50
13	B	101	SPO	C14-C12	2.32	1.38	1.35
13	O	102	SPO	C32-C33	2.32	1.38	1.33
8	D	101	BCL	O1A-CGA	-2.31	1.15	1.22
8	A	101	BCL	O1A-CGA	-2.31	1.15	1.22
13	F	102	SPO	C14-C12	2.31	1.38	1.35
11	L	305	U10	C1-C2	-2.31	1.39	1.47
13	W	103	SPO	C8-C7	2.30	1.55	1.50
10	H	301	PC1	P-O11	2.30	1.68	1.59
13	O	104	SPO	C24-C23	2.30	1.55	1.50
13	P	101	SPO	C36-C37	2.30	1.57	1.50
13	U	102	SPO	C14-C12	2.30	1.38	1.35
13	F	102	SPO	C24-C23	2.29	1.55	1.50
13	X	101	SPO	C8-C7	2.29	1.55	1.50
13	P	101	SPO	C14-C12	2.29	1.38	1.35
11	L	308	U10	C1-C2	-2.29	1.39	1.47
11	L	305	U10	C6-C1	2.29	1.39	1.35
13	8	102	SPO	C8-C7	2.29	1.55	1.50
10	H	302	PC1	C14-N	-2.29	1.43	1.50
13	W	103	SPO	C30-C31	2.28	1.61	1.53
10	H	303	PC1	P-O13	2.28	1.68	1.59
13	G	101	SPO	C36-C37	2.28	1.57	1.50
13	3	104	SPO	C18-C17	2.27	1.55	1.50
13	T	102	SPO	C14-C12	2.27	1.38	1.35
10	A	102	PC1	P-O11	2.26	1.68	1.59
10	L	304	PC1	P-O13	2.26	1.68	1.59
11	Y	501	U10	C1-C2	-2.25	1.39	1.47
8	W	102	BCL	O1A-CGA	-2.25	1.15	1.22
13	D	102	SPO	C8-C7	2.24	1.55	1.50
10	H	302	PC1	P-O13	2.24	1.68	1.59
10	L	306	PC1	P-O11	2.23	1.68	1.59
8	3	101	BCL	C4B-NB	2.23	1.37	1.35
13	X	101	SPO	C30-C31	2.22	1.61	1.53
13	B	101	SPO	C24-C23	2.22	1.55	1.50
13	M	405	SPO	C30-C31	2.21	1.61	1.53
13	I	102	SPO	C8-C7	2.21	1.55	1.50
10	A	104	PC1	P-O13	2.21	1.68	1.59
10	D	104	PC1	P-O11	2.21	1.68	1.59
13	D	103	SPO	C24-C23	2.20	1.55	1.50
10	A	102	PC1	C14-N	-2.19	1.43	1.50
10	H	301	PC1	C14-N	-2.19	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	303	PC1	C14-N	-2.19	1.43	1.50
10	W	101	PC1	P-O11	2.19	1.68	1.59
13	U	104	SPO	C8-C7	2.18	1.55	1.50
8	M	402	BCL	O1A-CGA	-2.18	1.16	1.22
13	U	102	SPO	C24-C23	2.18	1.55	1.50
8	U	101	BCL	O1A-CGA	-2.17	1.16	1.22
13	G	101	SPO	C29-C28	2.17	1.56	1.50
13	V	101	SPO	C14-C12	2.17	1.38	1.35
10	W	101	PC1	C14-N	-2.16	1.43	1.50
13	3	102	SPO	C35-C36	2.16	1.60	1.53
8	L	302	BCL	O1A-CGA	-2.16	1.16	1.22
10	L	306	PC1	C14-N	-2.16	1.43	1.50
10	D	104	PC1	C14-N	-2.16	1.43	1.50
13	U	104	SPO	C14-C12	2.15	1.38	1.35
10	L	304	PC1	C14-N	-2.15	1.43	1.50
8	N	101	BCL	O1A-CGA	-2.15	1.16	1.22
10	L	304	PC1	P-O11	2.15	1.68	1.59
13	T	102	SPO	C36-C37	2.14	1.57	1.50
10	L	306	PC1	P-O13	2.14	1.68	1.59
13	D	103	SPO	C30-C31	2.14	1.60	1.53
10	D	104	PC1	P-O13	2.13	1.67	1.59
13	X	101	SPO	C14-C12	2.13	1.38	1.35
13	0	101	SPO	C36-C37	2.13	1.57	1.50
13	B	101	SPO	C30-C31	2.12	1.60	1.53
13	E	102	SPO	C18-C17	2.12	1.55	1.50
14	H	304	CDL	OA6-CA4	-2.12	1.41	1.46
13	O	104	SPO	C36-C37	2.12	1.57	1.50
13	G	101	SPO	C35-C36	2.11	1.60	1.53
10	A	104	PC1	C14-N	-2.11	1.43	1.50
13	3	102	SPO	C29-C28	2.11	1.56	1.50
13	X	101	SPO	C24-C23	2.10	1.55	1.50
13	0	101	SPO	C8-C7	2.10	1.55	1.50
13	B	101	SPO	C8-C7	2.08	1.55	1.50
13	0	101	SPO	C14-C12	2.08	1.38	1.35
13	G	101	SPO	C24-C23	2.08	1.55	1.50
13	I	102	SPO	C36-C37	2.07	1.57	1.50
13	9	102	SPO	C36-C37	2.07	1.57	1.50
13	J	101	SPO	C32-C33	2.06	1.37	1.33
10	H	302	PC1	P-O11	2.06	1.67	1.59
13	V	101	SPO	C8-C7	2.06	1.55	1.50
13	V	101	SPO	C24-C23	2.06	1.55	1.50
13	D	102	SPO	C36-C37	2.05	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	306	PC1	C22-C21	2.04	1.56	1.50
13	D	103	SPO	C14-C12	2.04	1.38	1.35
13	V	101	SPO	C36-C37	2.04	1.57	1.50
13	W	103	SPO	C36-C37	2.02	1.57	1.50
8	1	101	BCL	C4B-NB	2.02	1.37	1.35
13	T	101	SPO	C36-C37	2.01	1.57	1.50
13	N	102	SPO	C36-C37	2.01	1.57	1.50
8	O	103	BCL	O1A-CGA	-2.01	1.16	1.22
13	J	103	SPO	C35-C36	2.00	1.60	1.53

All (1271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	V	101	SPO	C29-C28-C30	-49.64	31.77	115.27
13	J	103	SPO	C34-C33-C35	-32.50	60.59	115.27
13	N	102	SPO	C24-C23-C22	31.82	167.50	122.92
13	3	104	SPO	C34-C33-C35	-31.75	61.87	115.27
13	O	104	SPO	C24-C23-C22	31.71	167.35	122.92
13	X	101	SPO	C24-C23-C22	31.67	167.28	122.92
13	9	102	SPO	C24-C23-C22	31.61	167.20	122.92
13	B	101	SPO	C24-C23-C22	31.51	167.06	122.92
13	T	101	SPO	C24-C23-C22	31.31	166.79	122.92
13	F	102	SPO	C24-C23-C22	31.20	166.63	122.92
13	D	102	SPO	C24-C23-C22	31.14	166.54	122.92
13	8	102	SPO	C24-C23-C25	-30.98	69.26	118.08
13	V	101	SPO	C24-C23-C22	30.97	166.30	122.92
13	J	101	SPO	C24-C23-C22	30.24	165.29	122.92
13	I	102	SPO	C24-C23-C22	30.04	165.01	122.92
13	U	102	SPO	C24-C23-C22	29.78	164.63	122.92
13	G	101	SPO	C24-C23-C22	29.53	164.28	122.92
13	W	103	SPO	C24-C23-C22	29.48	164.21	122.92
13	P	101	SPO	C24-C23-C22	29.29	163.96	122.92
13	P	101	SPO	C34-C33-C35	-29.10	66.31	115.27
13	U	104	SPO	C24-C23-C22	28.87	163.36	122.92
13	0	101	SPO	C24-C23-C22	28.73	163.17	122.92
13	3	102	SPO	C24-C23-C22	28.68	163.10	122.92
13	G	101	SPO	C29-C28-C30	-28.30	67.67	115.27
13	3	104	SPO	C24-C23-C22	28.12	162.32	122.92
13	M	405	SPO	C24-C23-C22	27.97	162.11	122.92
13	T	102	SPO	C24-C23-C22	27.97	162.11	122.92
13	O	102	SPO	C24-C23-C22	27.86	161.95	122.92
13	E	102	SPO	C24-C23-C22	27.78	161.84	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	J	103	SPO	C24-C23-C22	26.92	160.63	122.92
13	D	103	SPO	C21-C22-C23	-26.30	89.77	127.31
13	8	102	SPO	C5-C6-C7	25.79	164.86	125.89
13	J	101	SPO	C34-C33-C35	-25.70	72.04	115.27
13	U	104	SPO	C35-C33-C32	25.50	172.71	121.12
13	M	405	SPO	C35-C33-C32	25.17	172.06	121.12
13	D	103	SPO	C35-C33-C32	24.87	171.44	121.12
13	G	101	SPO	C24-C23-C25	-24.56	79.37	118.08
13	G	101	SPO	C21-C22-C23	-24.28	92.66	127.31
13	F	102	SPO	C35-C33-C32	24.10	169.88	121.12
13	3	102	SPO	C29-C28-C30	-24.09	74.74	115.27
13	G	101	SPO	C35-C33-C32	23.99	169.65	121.12
13	E	102	SPO	C35-C33-C32	23.91	169.51	121.12
13	T	101	SPO	C35-C33-C32	23.88	169.43	121.12
13	D	103	SPO	C24-C23-C22	23.80	156.27	122.92
13	N	102	SPO	C34-C33-C35	-23.75	75.31	115.27
13	N	102	SPO	C35-C33-C32	23.75	169.17	121.12
13	8	102	SPO	C35-C33-C32	23.63	168.94	121.12
13	3	102	SPO	C35-C33-C32	23.34	168.36	121.12
13	D	102	SPO	C35-C33-C32	23.30	168.27	121.12
13	0	101	SPO	C24-C23-C25	-23.28	81.40	118.08
13	U	102	SPO	C35-C33-C32	23.27	168.22	121.12
13	0	101	SPO	C5-C6-C7	23.21	160.97	125.89
13	X	101	SPO	C35-C33-C32	23.17	168.01	121.12
13	B	101	SPO	C35-C33-C32	23.09	167.84	121.12
13	8	102	SPO	C25-C23-C22	-22.95	83.73	118.94
13	T	102	SPO	C35-C33-C32	22.94	167.54	121.12
13	O	102	SPO	C34-C33-C35	-22.78	76.95	115.27
13	D	103	SPO	C5-C6-C7	22.64	160.10	125.89
13	T	102	SPO	C24-C23-C25	-22.62	82.44	118.08
13	W	103	SPO	C35-C33-C32	22.48	166.61	121.12
13	0	101	SPO	C35-C33-C32	22.35	166.34	121.12
13	V	101	SPO	C35-C33-C32	22.25	166.15	121.12
13	I	102	SPO	C35-C33-C32	22.18	165.99	121.12
13	X	101	SPO	C24-C23-C25	-22.14	83.20	118.08
13	V	101	SPO	C24-C23-C25	-21.78	83.76	118.08
13	M	405	SPO	C34-C33-C35	-21.70	78.76	115.27
13	O	104	SPO	C24-C23-C25	-21.47	84.24	118.08
13	V	101	SPO	C5-C6-C7	21.45	158.30	125.89
13	8	102	SPO	C24-C23-C22	21.41	152.92	122.92
13	9	102	SPO	C24-C23-C25	-21.32	84.48	118.08
13	3	104	SPO	C24-C23-C25	-21.18	84.71	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	101	SPO	C24-C23-C25	-21.09	84.85	118.08
13	O	104	SPO	C35-C33-C32	21.08	163.77	121.12
13	9	102	SPO	C35-C33-C32	20.92	163.45	121.12
13	T	102	SPO	C20-C21-C22	-20.87	80.72	123.47
13	U	104	SPO	C34-C33-C35	-20.75	80.36	115.27
13	0	101	SPO	C21-C22-C23	-20.72	97.74	127.31
13	D	103	SPO	C34-C33-C35	-20.60	80.61	115.27
13	J	101	SPO	C29-C28-C30	-20.47	80.84	115.27
13	F	102	SPO	C5-C6-C7	20.28	156.53	125.89
13	J	103	SPO	C5-C6-C7	20.27	156.53	125.89
13	P	101	SPO	C24-C23-C25	-20.24	86.18	118.08
13	0	101	SPO	C20-C19-C17	-20.16	98.54	127.31
13	F	102	SPO	C24-C23-C25	-20.08	86.44	118.08
13	G	101	SPO	C5-C6-C7	19.96	156.06	125.89
13	E	102	SPO	C5-C6-C7	19.95	156.03	125.89
13	U	102	SPO	C5-C6-C7	19.67	155.62	125.89
13	3	102	SPO	C5-C6-C7	19.59	155.49	125.89
13	W	103	SPO	C5-C6-C7	19.48	155.33	125.89
13	B	101	SPO	C24-C23-C25	-19.48	87.39	118.08
13	I	102	SPO	C5-C6-C7	19.40	155.21	125.89
13	P	101	SPO	C5-C6-C7	19.36	155.14	125.89
13	E	102	SPO	C34-C33-C35	-19.23	82.93	115.27
13	T	101	SPO	C34-C33-C35	-19.20	82.96	115.27
13	9	102	SPO	C5-C6-C7	19.17	154.87	125.89
13	D	102	SPO	C24-C23-C25	-19.16	87.88	118.08
13	J	101	SPO	C24-C23-C25	-19.15	87.91	118.08
13	M	405	SPO	C5-C6-C7	19.09	154.74	125.89
13	N	102	SPO	C24-C23-C25	-19.02	88.11	118.08
13	V	101	SPO	C21-C22-C23	-18.96	100.25	127.31
13	8	102	SPO	C34-C33-C35	-18.92	83.44	115.27
13	J	103	SPO	C21-C22-C23	-18.86	100.39	127.31
13	F	102	SPO	C34-C33-C35	-18.84	83.57	115.27
13	J	103	SPO	C24-C23-C25	-18.84	88.39	118.08
13	J	101	SPO	C29-C28-C27	18.80	171.11	122.59
13	9	102	SPO	C29-C28-C30	-18.73	83.77	115.27
13	X	101	SPO	C5-C6-C7	18.66	154.08	125.89
13	J	101	SPO	C21-C22-C23	-18.54	100.86	127.31
13	D	103	SPO	C20-C19-C17	-18.52	100.88	127.31
13	D	102	SPO	C34-C33-C35	-18.47	84.20	115.27
13	X	101	SPO	C34-C33-C35	-18.39	84.33	115.27
13	O	102	SPO	C5-C6-C7	18.34	153.60	125.89
13	B	101	SPO	C29-C28-C27	18.34	169.92	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	U	102	SPO	C34-C33-C35	-18.30	84.49	115.27
13	I	102	SPO	C24-C23-C25	-18.26	89.31	118.08
13	U	104	SPO	C5-C6-C7	18.19	153.38	125.89
13	U	102	SPO	C24-C23-C25	-18.17	89.45	118.08
13	T	102	SPO	C5-C6-C7	18.12	153.28	125.89
13	W	103	SPO	C29-C28-C27	18.11	169.35	122.59
13	E	102	SPO	C13-C12-C11	-18.06	89.62	118.08
13	T	102	SPO	C34-C33-C35	-18.05	84.90	115.27
13	W	103	SPO	C24-C23-C25	-17.98	89.75	118.08
13	X	101	SPO	C21-C22-C23	-17.97	101.67	127.31
13	9	102	SPO	C29-C28-C27	17.96	168.94	122.59
13	B	101	SPO	C5-C6-C7	17.95	153.01	125.89
13	D	102	SPO	C29-C28-C27	17.94	168.89	122.59
13	W	103	SPO	C29-C28-C30	-17.93	85.10	115.27
13	O	104	SPO	C5-C6-C7	17.92	152.97	125.89
13	O	102	SPO	C29-C28-C30	-17.89	85.17	115.27
13	T	101	SPO	C29-C28-C27	17.85	168.67	122.59
13	O	102	SPO	C35-C33-C32	17.84	157.23	121.12
13	M	405	SPO	C29-C28-C27	17.84	168.64	122.59
13	B	101	SPO	C29-C28-C30	-17.76	85.39	115.27
13	U	102	SPO	C29-C28-C27	17.68	168.24	122.59
13	3	102	SPO	C34-C33-C35	-17.65	85.58	115.27
13	T	101	SPO	C5-C6-C7	17.60	152.49	125.89
13	O	104	SPO	C29-C28-C27	17.59	167.99	122.59
13	M	405	SPO	C29-C28-C30	-17.54	85.77	115.27
13	O	102	SPO	C29-C28-C27	17.44	167.61	122.59
13	I	102	SPO	C29-C28-C27	17.43	167.58	122.59
13	3	104	SPO	C21-C22-C23	-17.41	102.46	127.31
13	F	102	SPO	C29-C28-C27	17.39	167.49	122.59
13	D	102	SPO	C5-C6-C7	17.38	152.15	125.89
13	O	102	SPO	C21-C22-C23	-17.37	102.52	127.31
13	T	101	SPO	C21-C22-C23	-17.35	102.55	127.31
13	G	101	SPO	C20-C19-C17	-17.34	102.56	127.31
13	0	101	SPO	C29-C28-C27	17.33	167.32	122.59
13	E	102	SPO	C24-C23-C25	-17.32	90.79	118.08
13	X	101	SPO	C29-C28-C30	-17.31	86.15	115.27
13	B	101	SPO	C34-C33-C35	-17.29	86.18	115.27
13	N	102	SPO	C5-C6-C7	17.27	151.99	125.89
13	J	103	SPO	C29-C28-C27	17.25	167.10	122.59
13	P	101	SPO	C29-C28-C30	-17.12	86.48	115.27
13	M	405	SPO	C24-C23-C25	-17.10	91.13	118.08
13	D	103	SPO	C29-C28-C27	17.08	166.69	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	102	SPO	C18-C17-C16	-17.07	91.18	118.08
13	U	104	SPO	C24-C23-C25	-17.06	91.20	118.08
13	P	101	SPO	C21-C22-C23	-17.03	103.00	127.31
13	N	102	SPO	C29-C28-C27	17.01	166.50	122.59
13	3	104	SPO	C29-C28-C27	16.97	166.40	122.59
13	J	103	SPO	C35-C33-C32	16.95	155.41	121.12
13	X	101	SPO	C29-C28-C27	16.94	166.31	122.59
13	J	101	SPO	C35-C33-C32	16.92	155.35	121.12
13	B	101	SPO	C21-C22-C23	-16.91	103.18	127.31
13	O	102	SPO	C34-C33-C32	-16.85	80.44	123.68
13	D	103	SPO	C24-C23-C25	-16.85	91.53	118.08
13	P	101	SPO	C29-C28-C27	16.85	166.07	122.59
13	U	104	SPO	C29-C28-C27	16.70	165.69	122.59
13	9	102	SPO	C21-C22-C23	-16.64	103.57	127.31
13	T	102	SPO	C29-C28-C27	16.50	165.18	122.59
13	3	104	SPO	C35-C33-C32	16.49	154.48	121.12
13	3	104	SPO	C8-C7-C6	-16.47	92.13	118.08
13	J	103	SPO	C29-C28-C30	-16.32	87.82	115.27
13	0	101	SPO	C34-C33-C35	-16.31	87.83	115.27
13	3	102	SPO	C21-C22-C23	-16.19	104.21	127.31
13	3	104	SPO	C29-C28-C30	-16.17	88.06	115.27
13	E	102	SPO	C29-C28-C27	16.17	164.34	122.59
13	0	101	SPO	C15-C14-C12	-16.17	104.24	127.31
13	I	102	SPO	C21-C22-C23	-16.16	104.25	127.31
13	3	102	SPO	C24-C23-C25	-16.14	92.65	118.08
13	I	102	SPO	C34-C33-C35	-16.11	88.17	115.27
13	O	104	SPO	C21-C22-C23	-16.10	104.34	127.31
13	8	102	SPO	C29-C28-C27	16.02	163.94	122.59
13	P	101	SPO	C34-C33-C32	-16.02	82.59	123.68
13	T	102	SPO	C8-C7-C6	-16.01	92.85	118.08
13	O	104	SPO	C29-C28-C30	-16.01	88.33	115.27
13	T	101	SPO	C20-C21-C22	-16.00	90.70	123.47
13	O	102	SPO	C24-C23-C25	-15.99	92.88	118.08
13	8	102	SPO	C29-C28-C30	-15.98	88.40	115.27
13	8	102	SPO	C18-C17-C16	-15.96	92.93	118.08
13	0	101	SPO	C29-C28-C30	-15.94	88.45	115.27
13	N	102	SPO	C8-C7-C6	-15.88	93.06	118.08
13	W	103	SPO	C21-C22-C23	-15.84	104.70	127.31
13	T	101	SPO	C29-C28-C30	-15.78	88.72	115.27
13	U	102	SPO	C21-C22-C23	-15.76	104.81	127.31
13	D	102	SPO	C29-C28-C30	-15.76	88.76	115.27
13	0	101	SPO	C13-C12-C11	-15.75	93.27	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	J	101	SPO	C34-C33-C32	-15.74	83.31	123.68
13	D	102	SPO	C21-C22-C23	-15.70	104.91	127.31
13	3	102	SPO	C29-C28-C27	15.63	162.93	122.59
13	J	103	SPO	C13-C12-C11	-15.61	93.49	118.08
13	F	102	SPO	C21-C22-C23	-15.52	105.16	127.31
13	G	101	SPO	C34-C33-C35	-15.45	89.28	115.27
13	F	102	SPO	C29-C28-C30	-15.43	89.32	115.27
13	8	102	SPO	C20-C21-C22	-15.41	91.91	123.47
13	G	101	SPO	C13-C12-C11	-15.39	93.82	118.08
13	0	101	SPO	C8-C7-C6	-15.19	94.15	118.08
13	W	103	SPO	C34-C33-C35	-15.16	89.77	115.27
13	U	104	SPO	C29-C28-C30	-15.15	89.78	115.27
13	O	104	SPO	C34-C33-C35	-15.11	89.85	115.27
13	T	102	SPO	C29-C28-C30	-14.85	90.28	115.27
13	M	405	SPO	C21-C22-C23	-14.77	106.23	127.31
13	E	102	SPO	C29-C28-C30	-14.76	90.44	115.27
13	N	102	SPO	C29-C28-C30	-14.75	90.46	115.27
13	3	104	SPO	C6-C7-C9	14.67	141.45	118.94
13	B	101	SPO	C8-C7-C6	-14.65	94.99	118.08
13	D	103	SPO	C8-C7-C6	-14.62	95.04	118.08
13	D	103	SPO	C29-C28-C30	-14.50	90.87	115.27
13	8	102	SPO	C13-C12-C11	-14.41	95.37	118.08
13	E	102	SPO	C21-C22-C23	-14.39	106.77	127.31
13	I	102	SPO	C20-C21-C22	-14.23	94.33	123.47
13	3	102	SPO	C20-C21-C22	-14.23	94.33	123.47
13	J	101	SPO	C20-C21-C22	-14.23	94.33	123.47
13	G	101	SPO	C29-C28-C27	14.18	159.20	122.59
13	I	102	SPO	C29-C28-C30	-14.18	91.42	115.27
13	E	102	SPO	C8-C7-C6	-14.17	95.76	118.08
13	J	103	SPO	C20-C19-C17	-14.17	107.09	127.31
13	U	104	SPO	C8-C7-C6	-14.06	95.93	118.08
13	T	101	SPO	C8-C7-C6	-13.90	96.17	118.08
13	U	102	SPO	C29-C28-C30	-13.88	91.92	115.27
13	V	101	SPO	C27-C26-C25	-13.86	79.97	123.22
13	9	102	SPO	C20-C21-C22	-13.83	95.14	123.47
13	T	102	SPO	C15-C14-C12	-13.83	107.58	127.31
13	J	101	SPO	C5-C6-C7	13.81	146.77	125.89
13	U	104	SPO	C21-C22-C23	-13.78	107.65	127.31
13	9	102	SPO	C34-C33-C35	-13.77	92.10	115.27
13	F	102	SPO	C20-C21-C22	-13.75	95.31	123.47
13	B	101	SPO	C20-C21-C22	-13.74	95.33	123.47
13	P	101	SPO	C35-C33-C32	13.73	148.90	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	D	102	SPO	C8-C7-C6	-13.71	96.47	118.08
13	V	101	SPO	C34-C33-C35	-13.65	92.30	115.27
13	9	102	SPO	C8-C7-C6	-13.58	96.68	118.08
13	P	101	SPO	C8-C7-C6	-13.56	96.71	118.08
13	O	104	SPO	C8-C7-C6	-13.56	96.71	118.08
13	W	103	SPO	C8-C7-C6	-13.43	96.92	118.08
13	O	102	SPO	C20-C21-C22	-13.43	95.97	123.47
13	F	102	SPO	C8-C7-C6	-13.41	96.95	118.08
13	V	101	SPO	C8-C7-C6	-13.39	96.98	118.08
13	X	101	SPO	C8-C7-C6	-13.28	97.15	118.08
13	I	102	SPO	C8-C7-C6	-13.27	97.17	118.08
13	3	102	SPO	C8-C7-C6	-13.24	97.21	118.08
13	U	102	SPO	C20-C21-C22	-13.16	96.52	123.47
13	N	102	SPO	C13-C12-C11	-13.14	97.37	118.08
13	D	102	SPO	C20-C21-C22	-13.07	96.69	123.47
13	3	104	SPO	C5-C6-C7	13.07	145.64	125.89
13	V	101	SPO	C20-C21-C22	-13.06	96.73	123.47
13	J	103	SPO	C8-C7-C6	-13.04	97.53	118.08
13	G	101	SPO	C18-C17-C16	-12.99	97.60	118.08
13	X	101	SPO	C20-C21-C22	-12.93	96.98	123.47
13	W	103	SPO	C20-C21-C22	-12.92	97.02	123.47
13	O	102	SPO	C8-C7-C6	-12.89	97.77	118.08
13	G	101	SPO	C8-C7-C6	-12.83	97.86	118.08
13	U	102	SPO	C8-C7-C6	-12.74	98.00	118.08
13	0	101	SPO	C11-C12-C14	12.71	138.44	118.94
13	O	104	SPO	C20-C21-C22	-12.60	97.66	123.47
13	M	405	SPO	C18-C17-C16	-12.58	98.26	118.08
13	8	102	SPO	C8-C7-C6	-12.57	98.28	118.08
13	E	102	SPO	C20-C21-C22	-12.41	98.04	123.47
13	3	104	SPO	C20-C19-C17	-12.41	109.60	127.31
13	M	405	SPO	C8-C7-C6	-12.41	98.53	118.08
13	N	102	SPO	C10-C11-C12	-12.39	91.61	126.42
13	J	103	SPO	C13-C12-C14	12.38	140.26	122.92
13	8	102	SPO	C15-C16-C17	-12.31	91.84	126.42
13	8	102	SPO	C21-C22-C23	-12.27	109.80	127.31
13	E	102	SPO	C16-C17-C19	12.20	137.66	118.94
13	J	101	SPO	C8-C7-C6	-12.15	98.93	118.08
13	G	101	SPO	C15-C14-C12	-12.13	110.00	127.31
13	U	104	SPO	C18-C17-C16	-12.12	98.98	118.08
13	3	104	SPO	C34-C33-C32	-12.10	92.64	123.68
13	N	102	SPO	C20-C21-C22	-12.09	98.71	123.47
13	T	102	SPO	C13-C12-C11	-12.09	99.03	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	V	101	SPO	C21-C20-C19	-12.05	98.78	123.47
13	O	102	SPO	C21-C20-C19	-11.91	99.09	123.47
13	W	103	SPO	C13-C12-C11	-11.90	99.33	118.08
13	J	101	SPO	C21-C20-C19	-11.89	99.12	123.47
13	D	103	SPO	C15-C14-C12	-11.85	110.39	127.31
13	0	101	SPO	C18-C17-C16	-11.82	99.45	118.08
13	D	102	SPO	C21-C20-C19	-11.77	99.35	123.47
13	M	405	SPO	C20-C19-C17	-11.77	110.51	127.31
13	D	103	SPO	C10-C11-C12	-11.73	93.47	126.42
13	8	102	SPO	C16-C17-C19	11.70	136.90	118.94
13	U	104	SPO	C13-C12-C11	-11.66	99.71	118.08
13	U	104	SPO	C20-C21-C22	-11.65	99.61	123.47
13	X	101	SPO	C21-C20-C19	-11.61	99.69	123.47
13	B	101	SPO	C27-C26-C25	-11.56	87.13	123.22
13	N	102	SPO	C21-C22-C23	-11.48	110.93	127.31
13	J	103	SPO	C18-C17-C16	-11.46	100.02	118.08
13	E	102	SPO	C15-C16-C17	-11.41	94.36	126.42
13	T	101	SPO	C27-C26-C25	-11.41	87.61	123.22
13	0	101	SPO	C15-C16-C17	-11.40	94.40	126.42
13	8	102	SPO	C20-C19-C17	-11.39	111.06	127.31
13	J	103	SPO	C10-C11-C12	-11.37	94.47	126.42
13	I	102	SPO	C27-C26-C25	-11.32	87.88	123.22
13	J	103	SPO	C34-C33-C32	-11.25	94.83	123.68
13	G	101	SPO	C16-C17-C19	11.23	136.18	118.94
13	3	102	SPO	C30-C28-C27	-11.16	88.19	121.98
13	J	101	SPO	C31-C32-C33	-11.15	100.81	127.66
13	U	104	SPO	C21-C20-C19	-11.12	100.69	123.47
13	B	101	SPO	C21-C20-C19	-11.11	100.71	123.47
13	O	104	SPO	C21-C20-C19	-11.07	100.81	123.47
13	3	102	SPO	C21-C20-C19	-11.05	100.83	123.47
13	U	102	SPO	C27-C26-C25	-11.04	88.76	123.22
13	D	103	SPO	C15-C16-C17	-11.00	95.52	126.42
13	P	101	SPO	C20-C21-C22	-10.99	100.96	123.47
13	T	102	SPO	C10-C11-C12	-10.98	95.58	126.42
13	D	103	SPO	C18-C17-C16	-10.97	100.79	118.08
13	9	102	SPO	C27-C26-C25	-10.96	89.01	123.22
13	F	102	SPO	C27-C26-C25	-10.95	89.04	123.22
13	X	101	SPO	C27-C26-C25	-10.90	89.19	123.22
13	I	102	SPO	C21-C20-C19	-10.79	101.37	123.47
13	M	405	SPO	C20-C21-C22	-10.78	101.39	123.47
13	U	102	SPO	C18-C17-C16	-10.74	101.16	118.08
13	J	101	SPO	C27-C26-C25	-10.61	90.12	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	D	102	SPO	C27-C26-C25	-10.52	90.40	123.22
13	O	104	SPO	C27-C26-C25	-10.51	90.43	123.22
13	0	101	SPO	C6-C7-C9	10.48	135.02	118.94
13	P	101	SPO	C21-C20-C19	-10.47	102.03	123.47
13	G	101	SPO	C11-C12-C14	10.45	134.98	118.94
13	B	101	SPO	C18-C17-C16	-10.41	101.68	118.08
13	U	102	SPO	C21-C20-C19	-10.41	102.16	123.47
13	P	101	SPO	C13-C12-C11	-10.32	101.82	118.08
13	0	101	SPO	C16-C17-C19	10.30	134.75	118.94
13	W	103	SPO	C21-C20-C19	-10.23	102.51	123.47
13	P	101	SPO	C18-C17-C16	-10.22	101.98	118.08
13	0	101	SPO	C27-C26-C25	-10.20	91.39	123.22
13	U	102	SPO	C13-C12-C14	10.19	137.20	122.92
13	D	103	SPO	C16-C17-C19	10.18	134.56	118.94
13	U	102	SPO	C13-C12-C11	-10.16	102.06	118.08
13	N	102	SPO	C21-C20-C19	-10.14	102.71	123.47
13	N	102	SPO	C8-C7-C9	10.08	137.05	122.92
13	F	102	SPO	C21-C20-C19	-10.07	102.84	123.47
13	W	103	SPO	C18-C17-C16	-10.05	102.24	118.08
13	G	101	SPO	C30-C28-C27	-10.04	91.58	121.98
13	F	102	SPO	C13-C12-C11	-10.01	102.31	118.08
13	U	102	SPO	C18-C17-C19	10.00	136.93	122.92
13	9	102	SPO	C13-C12-C11	-9.97	102.37	118.08
13	T	102	SPO	C8-C7-C9	9.93	136.83	122.92
13	U	102	SPO	C8-C7-C9	9.91	136.81	122.92
13	9	102	SPO	C18-C17-C16	-9.91	102.46	118.08
13	W	103	SPO	C27-C26-C25	-9.85	92.49	123.22
13	N	102	SPO	C18-C17-C16	-9.82	102.60	118.08
13	N	102	SPO	C13-C12-C14	9.82	136.68	122.92
13	N	102	SPO	C34-C33-C32	-9.81	98.51	123.68
13	N	102	SPO	C25-C23-C22	-9.80	103.90	118.94
13	G	101	SPO	C27-C26-C25	-9.80	92.63	123.22
13	G	101	SPO	C15-C16-C17	-9.70	99.16	126.42
13	E	102	SPO	C11-C12-C14	9.68	133.79	118.94
13	3	104	SPO	C15-C14-C12	-9.64	113.55	127.31
13	3	102	SPO	C25-C23-C22	-9.60	104.20	118.94
13	V	101	SPO	C13-C12-C14	9.56	136.32	122.92
13	3	104	SPO	C13-C12-C11	-9.50	103.10	118.08
13	9	102	SPO	C21-C20-C19	-9.50	104.01	123.47
13	J	101	SPO	C8-C7-C9	9.49	136.22	122.92
13	9	102	SPO	C10-C11-C12	-9.48	99.78	126.42
13	8	102	SPO	C10-C11-C12	-9.48	99.78	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	102	SPO	C13-C12-C14	9.45	136.16	122.92
13	N	102	SPO	C27-C26-C25	-9.45	93.73	123.22
13	F	102	SPO	C18-C17-C16	-9.43	103.22	118.08
13	D	103	SPO	C8-C7-C9	9.33	135.99	122.92
13	3	102	SPO	C18-C17-C19	9.32	135.98	122.92
13	B	101	SPO	C18-C17-C19	9.31	135.96	122.92
13	U	102	SPO	C10-C11-C12	-9.26	100.40	126.42
13	J	103	SPO	C20-C21-C22	-9.25	104.52	123.47
13	W	103	SPO	C13-C12-C14	9.24	135.87	122.92
13	N	102	SPO	C15-C16-C17	-9.24	100.47	126.42
13	X	101	SPO	C18-C17-C16	-9.23	103.54	118.08
13	I	102	SPO	C18-C17-C19	9.21	135.83	122.92
13	I	102	SPO	C18-C17-C16	-9.20	103.58	118.08
13	X	101	SPO	C13-C12-C14	9.17	135.76	122.92
13	9	102	SPO	C13-C12-C14	9.14	135.73	122.92
13	O	104	SPO	C18-C17-C19	9.09	135.65	122.92
13	3	102	SPO	C18-C17-C16	-9.07	103.78	118.08
13	9	102	SPO	C18-C17-C19	9.05	135.60	122.92
13	B	101	SPO	C13-C12-C11	-9.01	103.88	118.08
13	O	102	SPO	C25-C23-C22	-8.98	105.16	118.94
13	O	104	SPO	C18-C17-C16	-8.98	103.94	118.08
13	U	104	SPO	C14-C15-C16	-8.96	95.24	123.22
13	V	101	SPO	C13-C12-C11	-8.96	103.96	118.08
13	0	101	SPO	C10-C9-C7	-8.90	114.61	127.31
13	F	102	SPO	C18-C17-C19	8.90	135.39	122.92
13	G	101	SPO	C34-C33-C32	-8.88	100.89	123.68
13	F	102	SPO	C8-C7-C9	8.86	135.33	122.92
13	9	102	SPO	C8-C7-C9	8.83	135.29	122.92
13	U	104	SPO	C25-C23-C22	-8.80	105.44	118.94
13	U	104	SPO	C13-C12-C14	8.80	135.25	122.92
13	D	102	SPO	C25-C23-C22	-8.79	105.46	118.94
13	T	102	SPO	C11-C12-C14	8.78	132.41	118.94
13	V	101	SPO	C29-C28-C27	-8.76	100.00	122.59
13	X	101	SPO	C13-C12-C11	-8.75	104.29	118.08
13	B	101	SPO	C25-C23-C22	-8.74	105.52	118.94
13	F	102	SPO	C13-C12-C14	8.74	135.16	122.92
13	V	101	SPO	C14-C15-C16	-8.72	95.99	123.22
13	E	102	SPO	C20-C19-C17	-8.72	114.87	127.31
13	I	102	SPO	C25-C23-C22	-8.72	105.57	118.94
13	I	102	SPO	C8-C7-C9	8.71	135.13	122.92
13	U	104	SPO	C18-C17-C19	8.71	135.13	122.92
13	F	102	SPO	C10-C11-C12	-8.71	101.95	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	102	SPO	C27-C26-C25	-8.70	96.06	123.22
13	J	103	SPO	C8-C7-C9	8.70	135.11	122.92
13	D	103	SPO	C20-C21-C22	-8.65	105.76	123.47
13	V	101	SPO	C34-C33-C32	-8.64	101.52	123.68
13	M	405	SPO	C8-C7-C9	8.60	134.97	122.92
13	J	101	SPO	C13-C12-C14	8.58	134.94	122.92
13	J	101	SPO	C14-C15-C16	-8.57	96.47	123.22
13	U	102	SPO	C25-C23-C22	-8.56	105.80	118.94
13	U	102	SPO	C15-C16-C17	-8.55	102.41	126.42
13	D	102	SPO	C18-C17-C19	8.53	134.87	122.92
13	M	405	SPO	C13-C12-C11	-8.53	104.64	118.08
13	X	101	SPO	C8-C7-C9	8.52	134.85	122.92
13	M	405	SPO	C13-C12-C14	8.51	134.85	122.92
14	M	406	CDL	OA8-CA6-CA4	8.51	133.21	108.43
13	O	102	SPO	C13-C12-C11	-8.49	104.70	118.08
13	T	101	SPO	C21-C20-C19	-8.49	106.08	123.47
13	X	101	SPO	C18-C17-C19	8.48	134.80	122.92
13	W	103	SPO	C8-C7-C9	8.47	134.79	122.92
13	W	103	SPO	C18-C17-C19	8.47	134.79	122.92
13	W	103	SPO	C25-C23-C22	-8.46	105.95	118.94
13	D	103	SPO	C11-C12-C14	8.43	131.88	118.94
13	I	102	SPO	C13-C12-C14	8.39	134.67	122.92
13	B	101	SPO	C13-C12-C14	8.38	134.67	122.92
13	3	102	SPO	C14-C15-C16	-8.38	97.07	123.22
13	O	102	SPO	C18-C17-C19	8.37	134.64	122.92
13	T	101	SPO	C18-C17-C16	-8.36	104.90	118.08
13	V	101	SPO	C18-C17-C19	8.36	134.64	122.92
13	P	101	SPO	C27-C26-C25	-8.34	97.20	123.22
13	O	102	SPO	C13-C12-C14	8.34	134.60	122.92
13	J	101	SPO	C13-C12-C11	-8.32	104.96	118.08
13	T	101	SPO	C14-C15-C16	-8.32	97.27	123.22
13	B	101	SPO	C8-C7-C9	8.31	134.56	122.92
13	I	102	SPO	C13-C12-C11	-8.29	105.01	118.08
13	D	103	SPO	C27-C26-C25	-8.29	97.35	123.22
13	T	101	SPO	C13-C12-C14	8.28	134.52	122.92
13	P	101	SPO	C18-C17-C19	8.27	134.51	122.92
13	3	102	SPO	C27-C26-C25	-8.26	97.45	123.22
13	T	102	SPO	C20-C19-C17	-8.25	115.54	127.31
13	O	102	SPO	C8-C7-C9	8.21	134.43	122.92
13	X	101	SPO	C14-C15-C16	-8.20	97.64	123.22
13	M	405	SPO	C27-C26-C25	-8.19	97.64	123.22
13	W	103	SPO	C10-C11-C12	-8.19	103.41	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	102	SPO	C9-C10-C11	-8.13	97.86	123.22
13	O	104	SPO	C8-C7-C9	8.12	134.30	122.92
13	T	101	SPO	C18-C17-C19	8.11	134.29	122.92
13	V	101	SPO	C18-C17-C16	-8.11	105.29	118.08
13	I	102	SPO	C10-C11-C12	-8.09	103.68	126.42
13	D	102	SPO	C13-C12-C14	8.07	134.23	122.92
13	O	104	SPO	C14-C15-C16	-8.06	98.06	123.22
13	8	102	SPO	C11-C12-C14	8.06	131.30	118.94
13	O	102	SPO	C18-C17-C16	-8.02	105.43	118.08
13	B	101	SPO	C15-C16-C17	-8.02	103.89	126.42
13	U	104	SPO	C27-C26-C25	-8.02	98.19	123.22
13	P	101	SPO	C13-C12-C14	7.98	134.10	122.92
13	D	102	SPO	C14-C15-C16	-7.98	98.31	123.22
13	J	103	SPO	C16-C17-C19	7.97	131.17	118.94
13	E	102	SPO	C27-C26-C25	-7.96	98.37	123.22
13	J	101	SPO	C10-C11-C12	-7.95	104.09	126.42
13	M	405	SPO	C25-C23-C22	-7.94	106.75	118.94
13	O	104	SPO	C13-C12-C14	7.93	134.03	122.92
13	J	101	SPO	C25-C23-C22	-7.92	106.79	118.94
13	W	103	SPO	C14-C15-C16	-7.92	98.51	123.22
13	J	103	SPO	C14-C15-C16	7.88	147.81	123.22
13	F	102	SPO	C25-C23-C22	-7.87	106.86	118.94
13	0	101	SPO	C20-C21-C22	-7.87	107.35	123.47
13	V	101	SPO	C8-C7-C9	7.85	133.92	122.92
14	H	304	CDL	OA8-CA6-CA4	7.84	131.26	108.43
13	W	103	SPO	C34-C33-C32	-7.83	103.58	123.68
13	D	102	SPO	C13-C12-C11	-7.83	105.74	118.08
13	X	101	SPO	C10-C11-C12	-7.81	104.49	126.42
13	M	405	SPO	C14-C15-C16	-7.80	98.88	123.22
13	O	104	SPO	C13-C12-C11	-7.79	105.80	118.08
13	E	102	SPO	C8-C7-C9	7.79	133.84	122.92
13	G	101	SPO	C10-C11-C12	-7.79	104.54	126.42
13	J	101	SPO	C18-C17-C19	7.78	133.83	122.92
13	P	101	SPO	C8-C7-C9	7.78	133.82	122.92
13	M	405	SPO	C10-C11-C12	-7.76	104.62	126.42
13	I	102	SPO	C14-C15-C16	-7.76	99.00	123.22
13	J	101	SPO	C18-C17-C16	-7.76	105.85	118.08
13	U	104	SPO	C10-C11-C12	-7.75	104.64	126.42
13	3	102	SPO	C13-C12-C14	7.73	133.76	122.92
13	M	405	SPO	C15-C16-C17	-7.73	104.70	126.42
13	U	104	SPO	C8-C7-C9	7.67	133.66	122.92
13	D	102	SPO	C18-C17-C16	-7.65	106.03	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	405	SPO	C34-C33-C32	-7.64	104.07	123.68
13	P	101	SPO	C14-C15-C16	-7.63	99.39	123.22
13	3	102	SPO	C8-C7-C9	7.63	133.61	122.92
13	O	102	SPO	C14-C15-C16	-7.62	99.43	123.22
13	9	102	SPO	C15-C16-C17	-7.58	105.12	126.42
13	O	102	SPO	C10-C11-C12	-7.58	105.14	126.42
13	T	101	SPO	C8-C7-C9	7.56	133.52	122.92
13	E	102	SPO	C25-C23-C22	-7.54	107.38	118.94
13	U	104	SPO	C9-C10-C11	-7.51	99.78	123.22
13	9	102	SPO	C34-C33-C32	-7.50	104.44	123.68
13	B	101	SPO	C6-C7-C9	7.50	130.44	118.94
13	O	102	SPO	C15-C16-C17	-7.48	105.39	126.42
13	D	102	SPO	C6-C7-C9	7.48	130.41	118.94
13	U	104	SPO	C6-C7-C9	7.47	130.40	118.94
13	E	102	SPO	C6-C7-C9	7.46	130.38	118.94
13	B	101	SPO	C10-C11-C12	-7.45	105.48	126.42
13	3	104	SPO	C20-C21-C22	-7.45	108.21	123.47
13	U	102	SPO	C14-C15-C16	-7.45	99.96	123.22
13	3	102	SPO	C13-C12-C11	-7.44	106.35	118.08
13	T	101	SPO	C13-C12-C11	-7.44	106.35	118.08
13	T	102	SPO	C6-C7-C9	7.42	130.32	118.94
13	T	101	SPO	C6-C7-C9	7.41	130.31	118.94
13	D	103	SPO	C10-C9-C7	-7.39	116.76	127.31
13	U	102	SPO	C30-C28-C27	-7.39	99.61	121.98
13	O	102	SPO	C27-C26-C25	-7.37	100.21	123.22
13	G	101	SPO	C8-C7-C9	7.36	133.23	122.92
13	0	101	SPO	C9-C10-C11	-7.35	100.29	123.22
13	9	102	SPO	C14-C15-C16	-7.33	100.33	123.22
13	8	102	SPO	C10-C9-C7	-7.31	116.87	127.31
13	G	101	SPO	C9-C10-C11	-7.30	100.44	123.22
13	D	102	SPO	C8-C7-C9	7.27	133.11	122.92
13	I	102	SPO	C15-C16-C17	-7.23	106.10	126.42
13	V	101	SPO	C10-C11-C12	-7.22	106.12	126.42
13	8	102	SPO	C13-C12-C14	7.22	133.03	122.92
13	O	104	SPO	C9-C10-C11	-7.21	100.71	123.22
13	F	102	SPO	C15-C16-C17	-7.21	106.16	126.42
13	0	101	SPO	C10-C11-C12	-7.20	106.19	126.42
13	X	101	SPO	C15-C16-C17	-7.18	106.24	126.42
13	F	102	SPO	C14-C15-C16	-7.17	100.84	123.22
13	M	405	SPO	C16-C17-C19	7.14	129.90	118.94
13	N	102	SPO	C6-C7-C9	7.12	129.86	118.94
13	O	102	SPO	C9-C10-C11	-7.06	101.20	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	I	102	SPO	C34-C33-C32	-7.06	105.58	123.68
13	3	102	SPO	C10-C11-C12	-7.04	106.63	126.42
13	3	102	SPO	C15-C16-C17	-7.04	106.65	126.42
13	F	102	SPO	C34-C33-C32	-7.03	105.64	123.68
13	D	102	SPO	C15-C16-C17	-7.02	106.70	126.42
13	0	101	SPO	C34-C33-C32	-7.01	105.68	123.68
13	9	102	SPO	C25-C23-C22	-7.01	108.18	118.94
13	3	102	SPO	C9-C10-C11	-7.00	101.36	123.22
13	O	104	SPO	C15-C16-C17	-6.99	106.77	126.42
13	8	102	SPO	C6-C7-C9	6.98	129.65	118.94
13	I	102	SPO	C30-C28-C27	-6.97	100.88	121.98
13	B	101	SPO	C34-C33-C32	-6.96	105.82	123.68
13	B	101	SPO	C14-C15-C16	-6.96	101.51	123.22
13	3	104	SPO	C10-C11-C12	-6.95	106.90	126.42
13	3	102	SPO	C34-C33-C32	-6.91	105.96	123.68
13	T	101	SPO	C25-C23-C22	-6.89	108.36	118.94
13	J	103	SPO	C27-C26-C25	-6.89	101.72	123.22
13	O	104	SPO	C25-C23-C22	-6.89	108.37	118.94
13	E	102	SPO	C21-C20-C19	-6.86	109.42	123.47
13	P	101	SPO	C6-C7-C9	6.86	129.47	118.94
13	P	101	SPO	C10-C11-C12	-6.80	107.32	126.42
13	3	104	SPO	C27-C26-C25	-6.79	102.02	123.22
13	P	101	SPO	C9-C10-C11	-6.79	102.03	123.22
13	3	104	SPO	C9-C10-C11	-6.79	102.03	123.22
13	O	104	SPO	C34-C33-C32	-6.78	106.29	123.68
13	3	104	SPO	C18-C17-C16	-6.76	107.42	118.08
13	U	102	SPO	C9-C10-C11	-6.75	102.15	123.22
13	D	103	SPO	C13-C12-C11	-6.74	107.45	118.08
13	D	102	SPO	C9-C10-C11	-6.73	102.22	123.22
13	V	101	SPO	C15-C16-C17	-6.72	107.53	126.42
13	V	101	SPO	C9-C10-C11	-6.69	102.33	123.22
13	3	102	SPO	C6-C7-C9	6.67	129.18	118.94
13	G	101	SPO	C20-C21-C22	-6.66	109.84	123.47
13	O	104	SPO	C10-C11-C12	-6.64	107.76	126.42
13	D	102	SPO	C10-C11-C12	-6.64	107.77	126.42
13	N	102	SPO	C20-C19-C17	-6.63	117.85	127.31
13	U	104	SPO	C34-C33-C32	-6.63	106.68	123.68
13	J	101	SPO	C15-C16-C17	-6.63	107.80	126.42
13	D	103	SPO	C34-C33-C32	-6.62	106.70	123.68
13	V	101	SPO	C6-C7-C9	6.62	129.09	118.94
13	D	102	SPO	C30-C28-C27	-6.60	102.01	121.98
13	T	101	SPO	C9-C10-C11	-6.59	102.64	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	101	SPO	C30-C28-C27	-6.59	102.03	121.98
13	T	101	SPO	C34-C33-C32	-6.57	106.81	123.68
13	J	101	SPO	C9-C10-C11	-6.57	102.71	123.22
13	P	101	SPO	C15-C16-C17	-6.56	107.99	126.42
13	T	101	SPO	C10-C11-C12	-6.56	107.99	126.42
13	O	104	SPO	C6-C7-C9	6.54	128.98	118.94
13	W	103	SPO	C9-C10-C11	-6.53	102.83	123.22
13	D	103	SPO	C30-C28-C27	-6.53	102.22	121.98
13	D	102	SPO	C34-C33-C32	-6.51	106.99	123.68
13	V	101	SPO	C31-C32-C33	-6.50	112.02	127.66
13	U	102	SPO	C34-C33-C32	-6.50	107.01	123.68
13	G	101	SPO	C6-C7-C9	6.49	128.91	118.94
13	8	102	SPO	C8-C7-C9	6.49	132.01	122.92
13	E	102	SPO	C10-C11-C12	-6.40	108.44	126.42
13	D	103	SPO	C6-C7-C9	6.40	128.76	118.94
13	E	102	SPO	C34-C33-C32	-6.35	107.39	123.68
13	M	405	SPO	C9-C10-C11	-6.33	103.45	123.22
13	N	102	SPO	C30-C28-C27	-6.31	102.87	121.98
13	T	102	SPO	C34-C33-C32	-6.30	107.52	123.68
13	X	101	SPO	C34-C33-C32	-6.30	107.53	123.68
13	8	102	SPO	C34-C33-C32	-6.27	107.60	123.68
13	I	102	SPO	C9-C10-C11	-6.24	103.74	123.22
13	X	101	SPO	C9-C10-C11	-6.22	103.80	123.22
13	F	102	SPO	C30-C28-C27	-6.21	103.19	121.98
13	U	104	SPO	C15-C16-C17	-6.20	109.00	126.42
13	M	405	SPO	C18-C17-C19	6.17	131.57	122.92
13	X	101	SPO	C25-C23-C22	-6.17	109.48	118.94
13	W	103	SPO	C15-C16-C17	-6.13	109.19	126.42
13	T	101	SPO	C15-C16-C17	-6.11	109.25	126.42
13	W	103	SPO	C6-C7-C9	6.09	128.28	118.94
13	O	104	SPO	C30-C28-C27	-6.06	103.63	121.98
13	0	101	SPO	C30-C28-C27	-6.04	103.71	121.98
13	D	102	SPO	C10-C9-C7	-6.03	118.71	127.31
13	B	101	SPO	C9-C10-C11	-6.02	104.43	123.22
13	J	101	SPO	C30-C28-C27	-6.01	103.78	121.98
13	B	101	SPO	C30-C28-C27	-6.00	103.81	121.98
13	P	101	SPO	C25-C23-C22	-5.98	109.76	118.94
13	9	102	SPO	C6-C7-C9	5.92	128.03	118.94
13	X	101	SPO	C6-C7-C9	5.90	128.00	118.94
13	8	102	SPO	C9-C10-C11	-5.90	104.79	123.22
13	3	104	SPO	C11-C12-C14	5.88	127.96	118.94
13	E	102	SPO	C18-C17-C19	5.88	131.15	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	V	101	SPO	C25-C23-C22	-5.87	109.94	118.94
13	U	104	SPO	C30-C28-C27	-5.86	104.23	121.98
13	J	103	SPO	C30-C28-C27	-5.84	104.30	121.98
13	F	102	SPO	C9-C10-C11	-5.78	105.17	123.22
13	8	102	SPO	C21-C20-C19	-5.78	111.63	123.47
13	T	102	SPO	C30-C28-C27	-5.78	104.49	121.98
13	O	102	SPO	C6-C7-C9	5.78	127.81	118.94
13	3	102	SPO	C26-C25-C23	-5.75	110.27	126.42
13	I	102	SPO	C6-C7-C9	5.71	127.70	118.94
13	F	102	SPO	C6-C7-C9	5.71	127.70	118.94
13	D	103	SPO	C31-C32-C33	-5.70	113.92	127.66
13	W	103	SPO	C30-C28-C27	-5.68	104.80	121.98
13	G	101	SPO	C26-C25-C23	-5.67	110.50	126.42
13	0	101	SPO	C8-C7-C9	5.64	130.82	122.92
13	8	102	SPO	C15-C14-C12	-5.63	119.27	127.31
13	9	102	SPO	C9-C10-C11	-5.62	105.67	123.22
13	M	405	SPO	C30-C28-C27	-5.59	105.06	121.98
13	T	102	SPO	C18-C17-C16	-5.58	109.28	118.08
13	E	102	SPO	C30-C28-C27	-5.54	105.22	121.98
13	O	104	SPO	C10-C9-C7	-5.51	119.44	127.31
13	G	101	SPO	C13-C12-C14	5.49	130.61	122.92
13	J	103	SPO	C6-C7-C9	5.48	127.35	118.94
8	U	103	BCL	C1-C2-C3	5.48	135.52	126.04
13	T	102	SPO	C26-C25-C23	-5.47	111.05	126.42
13	3	104	SPO	C30-C28-C27	-5.46	105.45	121.98
13	U	104	SPO	C10-C9-C7	-5.45	119.53	127.31
13	0	101	SPO	C21-C20-C19	5.44	134.63	123.47
13	J	101	SPO	C26-C25-C23	-5.38	111.30	126.42
13	3	102	SPO	C10-C9-C7	-5.34	119.69	127.31
13	N	102	SPO	C18-C17-C19	5.32	130.37	122.92
13	O	102	SPO	C26-C25-C23	-5.31	111.48	126.42
13	P	101	SPO	C26-C25-C23	-5.30	111.53	126.42
13	3	104	SPO	C26-C25-C23	-5.28	111.59	126.42
13	J	103	SPO	C25-C23-C22	-5.24	110.91	118.94
13	N	102	SPO	C10-C9-C7	-5.21	119.87	127.31
8	L	307	BCL	C1-C2-C3	5.21	135.05	126.04
13	T	101	SPO	C10-C9-C7	-5.18	119.92	127.31
13	J	103	SPO	C15-C14-C12	5.17	134.69	127.31
13	8	102	SPO	C18-C17-C19	5.16	130.15	122.92
13	N	102	SPO	C16-C17-C19	5.13	126.81	118.94
13	X	101	SPO	C26-C25-C23	-5.12	112.03	126.42
13	N	102	SPO	C26-C25-C23	-5.11	112.07	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3	104	SPO	C16-C17-C19	5.10	126.77	118.94
13	T	101	SPO	C26-C25-C23	-5.06	112.19	126.42
13	9	102	SPO	C30-C28-C27	-5.03	106.74	121.98
13	T	102	SPO	C14-C15-C16	4.96	138.71	123.22
8	R	101	BCL	C1-C2-C3	4.94	134.59	126.04
13	M	405	SPO	C6-C7-C9	4.92	126.50	118.94
13	3	104	SPO	C14-C15-C16	4.91	138.55	123.22
13	9	102	SPO	C26-C25-C23	-4.91	112.62	126.42
8	0	102	BCL	C1-C2-C3	4.89	134.50	126.04
13	O	104	SPO	C26-C25-C23	-4.88	112.70	126.42
13	O	102	SPO	C30-C28-C27	-4.88	107.22	121.98
13	P	101	SPO	C30-C28-C27	-4.86	107.25	121.98
13	G	101	SPO	C21-C20-C19	4.81	133.32	123.47
13	X	101	SPO	C30-C28-C27	-4.78	107.50	121.98
13	8	102	SPO	C30-C28-C27	-4.77	107.54	121.98
13	V	101	SPO	C10-C9-C7	-4.74	120.55	127.31
11	L	305	U10	C7-C8-C9	-4.74	118.90	126.79
13	T	102	SPO	C21-C20-C19	-4.74	113.77	123.47
14	M	406	CDL	OA6-CA5-C11	4.74	121.71	111.50
8	O	101	BCL	CMB-C2B-C1B	-4.64	121.33	128.46
13	J	103	SPO	C26-C25-C23	-4.62	113.42	126.42
9	L	303	BPB	CBC-CAC-C3C	-4.62	114.45	126.70
13	U	104	SPO	C31-C32-C33	-4.59	116.61	127.66
9	M	403	BPB	CBC-CAC-C3C	-4.59	114.53	126.70
13	N	102	SPO	C11-C12-C14	4.56	125.94	118.94
13	X	101	SPO	C31-C32-C33	-4.56	116.67	127.66
10	H	302	PC1	O21-C21-C22	4.54	121.28	111.50
13	P	101	SPO	C10-C9-C7	-4.50	120.89	127.31
8	M	402	BCL	CMB-C2B-C1B	-4.48	121.58	128.46
13	B	101	SPO	C31-C32-C33	-4.47	116.89	127.66
13	D	102	SPO	C26-C25-C23	-4.45	113.92	126.42
13	J	103	SPO	C11-C12-C14	4.45	125.76	118.94
8	L	307	BCL	CMB-C2B-C1B	-4.43	121.65	128.46
13	J	103	SPO	C9-C10-C11	-4.43	109.39	123.22
8	F	101	BCL	CMB-C2B-C1B	-4.43	121.66	128.46
8	Q	101	BCL	CMB-C2B-C1B	-4.43	121.66	128.46
13	D	103	SPO	C26-C25-C23	-4.41	114.04	126.42
10	A	102	PC1	O21-C21-C22	4.40	120.99	111.50
13	G	101	SPO	C10-C9-C7	-4.39	121.04	127.31
13	D	103	SPO	C25-C23-C22	-4.39	112.21	118.94
8	S	101	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
8	A	101	BCL	CMB-C2B-C1B	-4.35	121.77	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	U	104	SPO	C16-C17-C19	4.35	125.62	118.94
13	X	101	SPO	C36-C35-C33	-4.35	107.50	114.62
10	L	306	PC1	O21-C21-C22	4.34	120.84	111.50
8	L	301	BCL	CMB-C2B-C1B	-4.32	121.83	128.46
10	L	304	PC1	O21-C21-C22	4.31	120.79	111.50
8	U	101	BCL	CMB-C2B-C1B	-4.30	121.86	128.46
8	3	101	BCL	CMB-C2B-C1B	-4.29	121.86	128.46
8	1	101	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
14	H	304	CDL	OB6-CB5-C51	4.25	120.66	111.50
8	L	301	BCL	CAD-C3D-C4D	-4.24	106.10	108.47
8	D	101	BCL	CMB-C2B-C1B	-4.24	121.95	128.46
8	W	102	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
13	3	104	SPO	C13-C12-C14	4.20	128.80	122.92
10	A	104	PC1	O21-C21-C22	4.19	120.54	111.50
8	E	101	BCL	C1-C2-C3	4.18	133.28	126.04
10	W	101	PC1	O21-C21-C22	4.17	120.49	111.50
13	G	101	SPO	C31-C32-C33	-4.11	117.77	127.66
8	U	103	BCL	CMB-C2B-C1B	-4.10	122.16	128.46
8	I	101	BCL	CMB-C2B-C1B	-4.07	122.20	128.46
13	U	102	SPO	C6-C7-C9	4.07	125.18	118.94
10	H	303	PC1	O21-C21-O22	-4.06	120.40	125.57
8	L	302	BCL	CMB-C2B-C1B	-4.04	122.25	128.46
8	9	101	BCL	CMB-C2B-C1B	-4.01	122.30	128.46
8	O	103	BCL	CMB-C2B-C1B	-4.00	122.31	128.46
13	D	103	SPO	C1-C4-C5	-4.00	102.45	113.06
8	0	102	BCL	CMB-C2B-C1B	-3.97	122.36	128.46
14	H	304	CDL	OA6-CA5-C11	3.96	120.03	111.50
8	K	101	BCL	CMB-C2B-C1B	-3.95	122.39	128.46
13	3	104	SPO	C25-C23-C22	-3.93	112.91	118.94
8	7	101	BCL	C1-C2-C3	3.93	132.84	126.04
8	S	102	BCL	C1-C2-C3	3.93	132.83	126.04
13	U	104	SPO	C26-C25-C23	-3.92	115.41	126.42
13	0	101	SPO	C26-C25-C23	-3.91	115.43	126.42
13	B	101	SPO	C26-C25-C23	-3.91	115.43	126.42
8	8	101	BCL	CAD-C3D-C4D	-3.90	106.29	108.47
8	J	102	BCL	CMB-C2B-C1B	-3.89	122.48	128.46
8	E	101	BCL	C17-C16-C15	3.88	131.09	113.24
13	M	405	SPO	C10-C9-C7	-3.87	121.79	127.31
13	T	102	SPO	C13-C12-C14	3.86	128.34	122.92
8	S	102	BCL	CMB-C2B-C1B	-3.86	122.54	128.46
13	J	101	SPO	C6-C7-C9	3.85	124.85	118.94
8	E	101	BCL	CMB-C2B-C1B	-3.85	122.55	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	104	PC1	O21-C21-C22	3.85	119.79	111.50
13	J	101	SPO	C36-C35-C33	3.84	125.60	112.98
8	7	101	BCL	CMB-C2B-C1B	-3.83	122.58	128.46
13	U	104	SPO	C11-C12-C14	3.83	124.81	118.94
13	U	102	SPO	C26-C25-C23	-3.83	115.67	126.42
8	O	101	BCL	C4A-NA-C1A	3.81	108.42	106.71
8	9	101	BCL	C4A-NA-C1A	3.81	108.42	106.71
13	F	102	SPO	C26-C25-C23	-3.79	115.76	126.42
8	F	103	BCL	CMB-C2B-C1B	-3.79	122.64	128.46
8	R	101	BCL	CMB-C2B-C1B	-3.78	122.65	128.46
8	N	101	BCL	C1-C2-C3	3.78	132.58	126.04
8	E	101	BCL	C16-C15-C13	3.75	128.03	115.92
8	O	103	BCL	C1-C2-C3	-3.73	119.59	126.04
13	J	103	SPO	C18-C17-C19	3.71	128.12	122.92
11	L	308	U10	C22-C23-C24	-3.70	118.75	127.66
13	W	103	SPO	C11-C12-C14	3.69	124.61	118.94
8	N	101	BCL	CMB-C2B-C1B	-3.69	122.80	128.46
13	F	102	SPO	C31-C32-C33	-3.69	118.78	127.66
8	7	101	BCL	CAD-C3D-C4D	-3.68	106.42	108.47
8	3	103	BCL	CMB-C2B-C1B	-3.68	122.81	128.46
8	1	101	BCL	C4A-NA-C1A	3.67	108.36	106.71
8	Q	101	BCL	OBD-CAD-CBD	-3.67	120.65	125.89
13	O	102	SPO	C10-C9-C7	-3.66	122.08	127.31
8	R	101	BCL	CAD-C3D-C4D	-3.66	106.43	108.47
8	S	101	BCL	OBD-CAD-CBD	-3.65	120.67	125.89
13	O	102	SPO	C31-C32-C33	-3.63	118.91	127.66
8	U	101	BCL	C4A-NA-C1A	3.63	108.34	106.71
13	0	101	SPO	C13-C12-C14	3.60	127.96	122.92
8	C	101	BCL	CMB-C2B-C1B	-3.58	122.96	128.46
8	O	101	BCL	OBD-CAD-CBD	-3.58	120.78	125.89
8	3	101	BCL	OBD-CAD-CBD	-3.58	120.78	125.89
14	M	406	CDL	OB6-CB5-C51	3.56	119.18	111.50
8	K	101	BCL	OBD-CAD-CBD	-3.55	120.82	125.89
8	E	101	BCL	CAD-C3D-C4D	-3.55	106.49	108.47
8	D	101	BCL	OBD-CAD-CBD	-3.54	120.83	125.89
11	Y	501	U10	C12-C13-C14	-3.54	119.14	127.66
8	F	103	BCL	OBD-CAD-CBD	-3.52	120.86	125.89
13	W	103	SPO	C31-C32-C33	-3.52	119.18	127.66
8	R	101	BCL	OBD-CAD-CBD	-3.51	120.87	125.89
11	M	404	U10	C25-C24-C26	3.50	121.16	115.27
8	C	101	BCL	CAD-C3D-C4D	-3.50	106.52	108.47
8	W	102	BCL	OBD-CAD-CBD	-3.50	120.90	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	101	BCL	OBD-CAD-CBD	-3.49	120.91	125.89
8	A	103	BCL	CAD-C3D-C4D	-3.47	106.53	108.47
8	9	101	BCL	OBD-CAD-CBD	-3.47	120.94	125.89
13	G	101	SPO	C14-C15-C16	-3.47	112.40	123.22
10	H	301	PC1	O21-C21-C22	3.47	118.97	111.50
8	M	402	BCL	CAD-C3D-C4D	-3.46	106.54	108.47
8	S	102	BCL	OBD-CAD-CBD	-3.46	120.95	125.89
13	M	405	SPO	C26-C25-C23	-3.46	116.69	126.42
14	M	406	CDL	C57-C56-C55	3.46	131.99	114.42
8	F	101	BCL	OBD-CAD-CBD	-3.46	120.96	125.89
8	N	101	BCL	OBD-CAD-CBD	-3.45	120.97	125.89
8	7	101	BCL	OBD-CAD-CBD	-3.45	120.97	125.89
8	U	103	BCL	OBD-CAD-CBD	-3.44	120.97	125.89
8	C	101	BCL	C16-C15-C13	3.44	127.05	115.92
8	F	101	BCL	C4A-NA-C1A	3.44	108.25	106.71
13	B	101	SPO	C10-C9-C7	-3.44	122.40	127.31
8	8	101	BCL	OBD-CAD-CBD	-3.44	120.98	125.89
8	3	103	BCL	OBD-CAD-CBD	-3.43	121.00	125.89
8	F	103	BCL	O2A-C1-C2	-3.42	99.65	108.64
8	U	101	BCL	OBD-CAD-CBD	-3.41	121.02	125.89
8	O	101	BCL	CMB-C2B-C3B	3.40	131.04	124.68
13	U	102	SPO	C31-C32-C33	-3.40	119.48	127.66
8	I	101	BCL	OBD-CAD-CBD	-3.40	121.04	125.89
8	F	103	BCL	CAD-C3D-C4D	-3.39	106.58	108.47
8	L	302	BCL	OBD-CAD-CBD	-3.39	121.05	125.89
8	9	101	BCL	CAD-C3D-C4D	-3.38	106.58	108.47
8	E	101	BCL	OBD-CAD-CBD	-3.38	121.07	125.89
8	3	103	BCL	CAD-C3D-C4D	-3.38	106.59	108.47
8	0	102	BCL	OBD-CAD-CBD	-3.37	121.07	125.89
13	8	102	SPO	C31-C32-C33	-3.37	119.54	127.66
13	J	103	SPO	C10-C9-C7	-3.36	122.52	127.31
13	D	103	SPO	C36-C37-C38	-3.35	116.29	127.75
13	E	102	SPO	C31-C32-C33	-3.35	119.59	127.66
8	L	301	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
11	Y	501	U10	C17-C18-C19	-3.35	119.60	127.66
13	T	102	SPO	C31-C32-C33	-3.34	119.61	127.66
8	K	101	BCL	C4A-NA-C1A	3.33	108.20	106.71
8	A	103	BCL	CMB-C2B-C1B	-3.33	123.35	128.46
13	J	101	SPO	C10-C9-C7	-3.33	122.56	127.31
9	M	403	BPB	OBD-CAD-CBD	-3.32	120.94	125.82
8	1	102	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
8	F	103	BCL	C1-C2-C3	3.32	131.79	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	U	103	BCL	CAD-C3D-C4D	-3.32	106.62	108.47
8	J	102	BCL	CAD-C3D-C4D	-3.31	106.62	108.47
8	S	102	BCL	CAD-C3D-C4D	-3.31	106.62	108.47
13	I	102	SPO	C26-C25-C23	-3.31	117.11	126.42
13	D	103	SPO	C14-C15-C16	-3.31	112.90	123.22
8	C	101	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
8	1	101	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
8	W	102	BCL	C4A-NA-C1A	3.29	108.19	106.71
13	O	104	SPO	C31-C32-C33	-3.28	119.75	127.66
8	J	102	BCL	OBD-CAD-CBD	-3.28	121.21	125.89
13	J	101	SPO	C35-C36-C37	-3.28	101.10	111.88
8	M	402	BCL	CMB-C2B-C3B	3.28	130.81	124.68
8	Q	101	BCL	CMB-C2B-C3B	3.27	130.80	124.68
8	L	307	BCL	OBD-CAD-CBD	-3.27	121.22	125.89
8	A	103	BCL	C1-C2-C3	-3.26	120.40	126.04
8	D	101	BCL	C4A-NA-C1A	3.26	108.17	106.71
11	L	308	U10	C25-C24-C26	3.26	120.75	115.27
8	O	103	BCL	OBD-CAD-CBD	-3.26	121.24	125.89
8	M	402	BCL	CHA-C1A-NA	-3.25	118.95	126.40
8	W	102	BCL	CAD-C3D-C4D	-3.25	106.66	108.47
8	F	101	BCL	CMB-C2B-C3B	3.25	130.75	124.68
8	A	101	BCL	C4A-NA-C1A	3.25	108.17	106.71
11	L	305	U10	C30-C29-C31	3.24	120.73	115.27
8	L	302	BCL	C1-C2-C3	-3.24	120.43	126.04
8	U	101	BCL	CHA-C1A-NA	-3.24	118.98	126.40
8	L	302	BCL	CAD-C3D-C4D	-3.24	106.66	108.47
8	1	102	BCL	CMB-C2B-C1B	-3.24	123.49	128.46
13	V	101	SPO	C30-C28-C27	3.23	131.76	121.98
13	J	101	SPO	C20-C19-C17	-3.23	122.70	127.31
9	L	303	BPB	OBD-CAD-CBD	-3.22	121.09	125.82
13	E	102	SPO	C26-C25-C23	-3.22	117.38	126.42
13	T	102	SPO	C10-C9-C7	-3.22	122.72	127.31
13	M	405	SPO	C31-C32-C33	-3.21	119.92	127.66
8	I	101	BCL	C4A-NA-C1A	3.21	108.15	106.71
8	3	101	BCL	CAD-C3D-C4D	-3.21	106.68	108.47
8	L	307	BCL	CMB-C2B-C3B	3.20	130.67	124.68
8	U	101	BCL	CMB-C2B-C3B	3.20	130.66	124.68
8	D	101	BCL	CHA-C1A-NA	-3.19	119.09	126.40
8	S	101	BCL	CAD-C3D-C4D	-3.19	106.69	108.47
8	7	101	BCL	CHA-C1A-NA	-3.17	119.14	126.40
13	P	101	SPO	C11-C12-C14	3.17	123.80	118.94
8	A	103	BCL	OBD-CAD-CBD	-3.16	121.38	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	101	BCL	O2A-C1-C2	-3.16	100.33	108.64
13	T	102	SPO	C16-C17-C19	3.16	123.79	118.94
8	9	101	BCL	CHA-C1A-NA	-3.16	119.17	126.40
8	L	301	BCL	CMB-C2B-C3B	3.15	130.58	124.68
8	A	101	BCL	CMB-C2B-C3B	3.15	130.57	124.68
8	Q	101	BCL	CHA-C1A-NA	-3.15	119.19	126.40
8	O	101	BCL	CAD-C3D-C4D	-3.15	106.72	108.47
13	D	102	SPO	C31-C32-C33	-3.14	120.09	127.66
8	S	101	BCL	CMB-C2B-C3B	3.14	130.55	124.68
8	1	101	BCL	CAD-C3D-C4D	-3.14	106.72	108.47
8	M	402	BCL	C17-C16-C15	-3.13	98.84	113.24
8	F	101	BCL	CHA-C1A-NA	-3.13	119.23	126.40
8	Q	101	BCL	CAD-C3D-C4D	-3.13	106.72	108.47
8	S	102	BCL	C4A-NA-C1A	3.12	108.11	106.71
8	M	402	BCL	C4A-NA-C1A	3.12	108.11	106.71
8	1	102	BCL	C4A-NA-C1A	3.11	108.11	106.71
8	U	103	BCL	C16-C15-C13	3.11	125.96	115.92
8	D	101	BCL	CMB-C2B-C3B	3.10	130.47	124.68
8	O	103	BCL	CAD-C3D-C4D	-3.08	106.75	108.47
8	O	103	BCL	CHA-C1A-NA	-3.08	119.34	126.40
8	W	102	BCL	CMB-C2B-C3B	3.08	130.44	124.68
8	3	101	BCL	CMB-C2B-C3B	3.07	130.43	124.68
13	T	101	SPO	C20-C19-C17	-3.07	122.93	127.31
8	I	101	BCL	CHA-C1A-NA	-3.07	119.37	126.40
8	L	307	BCL	C4A-NA-C1A	3.07	108.08	106.71
8	L	307	BCL	C2A-C1A-CHA	3.06	129.21	123.86
8	A	101	BCL	CAD-C3D-C4D	-3.06	106.77	108.47
8	O	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
8	1	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
8	K	101	BCL	CHA-C1A-NA	-3.05	119.41	126.40
8	0	102	BCL	CAD-C3D-C4D	-3.05	106.77	108.47
8	7	101	BCL	C2A-C1A-CHA	3.05	129.19	123.86
11	M	404	U10	C35-C34-C36	3.05	120.39	115.27
8	3	101	BCL	CHA-C1A-NA	-3.05	119.42	126.40
8	8	101	BCL	CMB-C2B-C1B	-3.04	123.78	128.46
8	M	402	BCL	OBD-CAD-CBD	-3.04	121.55	125.89
8	A	103	BCL	CHA-C1A-NA	-3.04	119.43	126.40
13	I	102	SPO	C31-C30-C28	3.04	122.99	112.98
11	L	308	U10	C20-C19-C21	3.04	120.38	115.27
8	L	302	BCL	CHA-C1A-NA	-3.03	119.45	126.40
8	R	101	BCL	CHA-C1A-NA	-3.03	119.46	126.40
11	M	404	U10	C32-C33-C34	-3.03	120.37	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	305	U10	C25-C24-C26	3.03	120.36	115.27
8	K	101	BCL	CAD-C3D-C4D	-3.02	106.78	108.47
8	1	101	BCL	CMB-C2B-C3B	3.02	130.33	124.68
8	A	101	BCL	CHA-C1A-NA	-3.02	119.48	126.40
13	W	103	SPO	C10-C9-C7	-3.02	123.01	127.31
8	3	103	BCL	CHA-C1A-NA	-3.01	119.50	126.40
8	J	102	BCL	CHA-C1A-NA	-3.01	119.50	126.40
8	S	102	BCL	CHA-C1A-NA	-3.01	119.50	126.40
11	L	308	U10	C17-C18-C19	-3.01	120.41	127.66
8	S	101	BCL	C4A-NA-C1A	3.01	108.06	106.71
11	L	308	U10	C10-C9-C11	3.01	120.33	115.27
8	0	102	BCL	CHA-C1A-NA	-3.00	119.52	126.40
8	L	302	BCL	C2A-C1A-CHA	3.00	129.11	123.86
8	F	101	BCL	CAD-C3D-C4D	-3.00	106.80	108.47
8	U	103	BCL	CHA-C1A-NA	-2.99	119.56	126.40
8	N	101	BCL	CAD-C3D-C4D	-2.99	106.81	108.47
8	S	101	BCL	CHA-C1A-NA	-2.98	119.57	126.40
8	I	101	BCL	CMB-C2B-C3B	2.98	130.25	124.68
8	1	102	BCL	CAD-C3D-C4D	-2.98	106.81	108.47
8	M	402	BCL	C16-C15-C13	2.97	125.53	115.92
8	L	301	BCL	CHA-C1A-NA	-2.97	119.60	126.40
8	7	101	BCL	C17-C16-C15	2.96	126.86	113.24
13	N	102	SPO	C9-C10-C11	-2.96	113.97	123.22
8	7	101	BCL	CAA-CBA-CGA	2.96	121.90	113.25
8	1	102	BCL	CHA-C1A-NA	-2.96	119.62	126.40
8	L	302	BCL	CMB-C2B-C3B	2.95	130.20	124.68
8	9	101	BCL	C2A-C1A-CHA	2.95	129.02	123.86
8	W	102	BCL	CHA-C1A-NA	-2.95	119.65	126.40
8	E	101	BCL	C4A-NA-C1A	2.94	108.03	106.71
11	Y	501	U10	C15-C14-C16	2.94	120.22	115.27
8	F	103	BCL	CHA-C1A-NA	-2.94	119.67	126.40
8	N	101	BCL	C4A-NA-C1A	2.93	108.02	106.71
11	M	404	U10	C12-C13-C14	-2.93	120.61	127.66
13	W	103	SPO	C26-C25-C23	-2.93	118.19	126.42
8	C	101	BCL	CHA-C1A-NA	-2.93	119.70	126.40
8	U	103	BCL	CMB-C2B-C3B	2.92	130.15	124.68
13	D	103	SPO	C21-C20-C19	2.92	129.46	123.47
8	L	307	BCL	CHA-C1A-NA	-2.92	119.70	126.40
11	M	404	U10	C10-C9-C11	2.91	120.17	115.27
8	N	101	BCL	C16-C15-C13	-2.91	106.50	115.92
8	Q	101	BCL	C4A-NA-C1A	2.91	108.02	106.71
8	9	101	BCL	CMB-C2B-C3B	2.91	130.12	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
8	8	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
8	8	101	BCL	C4A-NA-C1A	2.90	108.01	106.71
13	P	101	SPO	C16-C17-C19	2.89	123.37	118.94
8	0	102	BCL	CMB-C2B-C3B	2.88	130.07	124.68
8	D	101	BCL	CAD-C3D-C4D	-2.88	106.86	108.47
8	I	101	BCL	CAD-C3D-C4D	-2.88	106.86	108.47
8	3	101	BCL	C4A-NA-C1A	2.88	108.00	106.71
11	L	308	U10	C12-C13-C14	-2.88	120.73	127.66
8	U	101	BCL	C2A-C1A-CHA	2.87	128.88	123.86
8	J	102	BCL	C4A-NA-C1A	2.87	108.00	106.71
8	J	102	BCL	CMB-C2B-C3B	2.86	130.04	124.68
8	L	302	BCL	C4A-NA-C1A	2.86	107.99	106.71
11	Y	501	U10	C25-C24-C26	2.86	120.08	115.27
8	A	103	BCL	O2A-C1-C2	-2.86	101.12	108.64
8	N	101	BCL	CHA-C1A-NA	-2.85	119.86	126.40
8	K	101	BCL	CMB-C2B-C3B	2.85	130.02	124.68
8	D	101	BCL	C2A-C1A-CHA	2.85	128.84	123.86
8	O	101	BCL	C2A-C1A-CHA	2.85	128.84	123.86
13	3	102	SPO	C31-C32-C33	-2.84	120.81	127.66
13	0	101	SPO	C31-C32-C33	-2.84	120.81	127.66
8	F	103	BCL	CMB-C2B-C3B	2.84	129.99	124.68
8	O	103	BCL	CMB-C2B-C3B	2.83	129.98	124.68
13	T	101	SPO	C31-C32-C33	-2.83	120.85	127.66
13	J	101	SPO	C40-C38-C39	2.83	120.84	114.60
8	L	301	BCL	C2A-C1A-CHA	2.82	128.79	123.86
8	U	101	BCL	CAD-C3D-C4D	-2.82	106.90	108.47
11	Y	501	U10	C7-C8-C9	-2.82	122.10	126.79
8	R	101	BCL	C4A-NA-C1A	2.82	107.97	106.71
8	L	301	BCL	C4A-NA-C1A	2.81	107.97	106.71
8	7	101	BCL	CMB-C2B-C3B	2.81	129.94	124.68
8	F	101	BCL	C2A-C1A-CHA	2.81	128.77	123.86
13	V	101	SPO	C26-C25-C23	-2.81	118.53	126.42
8	A	103	BCL	C2A-C1A-CHA	2.81	128.77	123.86
8	8	101	BCL	C11-C10-C8	-2.80	106.86	115.92
8	Q	101	BCL	C1C-NC-C4C	2.80	107.96	106.71
11	L	305	U10	C22-C23-C24	-2.79	120.93	127.66
8	E	101	BCL	CMB-C2B-C3B	2.79	129.90	124.68
11	M	404	U10	C22-C23-C24	-2.79	120.94	127.66
13	U	104	SPO	C20-C19-C17	-2.79	123.33	127.31
8	8	101	BCL	C6-C7-C8	-2.78	106.95	115.92
8	1	102	BCL	C2A-C1A-CHA	2.77	128.71	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	101	BCL	CMB-C2B-C3B	2.77	129.86	124.68
8	3	103	BCL	C4A-NA-C1A	2.77	107.95	106.71
8	A	101	BCL	C2A-C1A-CHA	2.76	128.69	123.86
13	T	102	SPO	C18-C17-C19	2.76	126.79	122.92
13	E	102	SPO	C10-C9-C7	-2.76	123.37	127.31
13	G	101	SPO	C36-C35-C33	2.75	122.04	112.98
8	S	102	BCL	CMB-C2B-C3B	2.75	129.83	124.68
8	L	307	BCL	CAD-C3D-C4D	-2.75	106.94	108.47
11	M	404	U10	C30-C29-C31	2.75	119.89	115.27
13	J	103	SPO	C40-C38-C39	2.75	120.67	114.60
14	H	304	CDL	OB8-CB7-C71	2.74	120.50	111.91
8	8	101	BCL	C2A-C1A-CHA	2.74	128.65	123.86
8	O	103	BCL	C2A-C1A-CHA	2.74	128.65	123.86
11	Y	501	U10	C20-C19-C21	2.73	119.86	115.27
8	N	101	BCL	CMB-C2B-C3B	2.73	129.78	124.68
13	8	102	SPO	C14-C15-C16	-2.72	114.71	123.22
8	S	102	BCL	C2A-C1A-CHA	2.72	128.62	123.86
13	9	102	SPO	C36-C35-C33	2.72	121.93	112.98
8	1	101	BCL	C2A-C1A-CHA	2.72	128.62	123.86
8	Q	101	BCL	C2A-C1A-CHA	2.71	128.60	123.86
8	C	101	BCL	C2A-C1A-CHA	2.71	128.60	123.86
10	H	302	PC1	O31-C31-C32	2.70	120.39	111.91
13	9	102	SPO	C31-C32-C33	-2.70	121.16	127.66
8	U	103	BCL	C4A-NA-C1A	2.70	107.92	106.71
13	3	104	SPO	C40-C38-C39	2.70	120.56	114.60
11	M	404	U10	C15-C14-C16	2.70	119.81	115.27
8	W	102	BCL	C1-C2-C3	-2.69	121.38	126.04
11	L	305	U10	C36-C34-C35	2.69	120.55	114.60
9	L	303	BPB	CMB-C2B-C3B	2.69	129.71	124.68
8	3	103	BCL	CMB-C2B-C3B	2.69	129.71	124.68
10	A	104	PC1	O31-C31-C32	2.68	120.33	111.91
8	I	101	BCL	C2A-C1A-CHA	2.68	128.55	123.86
8	C	101	BCL	CMB-C2B-C3B	2.68	129.69	124.68
8	O	103	BCL	C4A-NA-C1A	2.67	107.91	106.71
13	J	101	SPO	C36-C37-C38	-2.67	118.62	127.75
11	M	404	U10	C27-C28-C29	-2.67	121.23	127.66
8	U	103	BCL	C17-C16-C15	2.66	125.48	113.24
11	L	305	U10	C12-C13-C14	-2.66	121.27	127.66
8	0	102	BCL	C2A-C1A-CHA	2.65	128.49	123.86
8	F	103	BCL	C2A-C1A-CHA	2.65	128.49	123.86
8	W	102	BCL	C2A-C1A-CHA	2.64	128.47	123.86
8	C	101	BCL	C4A-NA-C1A	2.64	107.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	O	102	SPO	C20-C19-C17	-2.64	123.55	127.31
13	M	405	SPO	C1-C4-C5	-2.63	106.08	113.06
8	S	101	BCL	C2A-C1A-CHA	2.63	128.46	123.86
8	L	301	BCL	C1C-NC-C4C	2.63	107.89	106.71
11	M	404	U10	C17-C18-C19	-2.63	121.33	127.66
8	3	101	BCL	C2A-C1A-CHA	2.62	128.44	123.86
13	8	102	SPO	C26-C25-C23	2.62	133.76	126.42
14	H	304	CDL	OA8-CA7-C31	2.61	120.11	111.91
8	U	103	BCL	CMD-C2D-C3D	2.61	129.56	124.68
8	N	101	BCL	O2A-C1-C2	-2.61	101.78	108.64
13	B	101	SPO	C40-C38-C39	2.61	120.36	114.60
13	8	102	SPO	C27-C26-C25	-2.60	115.09	123.22
10	W	101	PC1	O31-C31-C32	2.60	120.08	111.91
8	K	101	BCL	C2A-C1A-CHA	2.60	128.41	123.86
10	A	102	PC1	O31-C31-C32	2.60	120.06	111.91
8	M	402	BCL	OBB-CAB-CBB	-2.59	114.34	120.17
8	C	101	BCL	CMD-C2D-C3D	2.58	129.50	124.68
8	7	101	BCL	CMD-C2D-C3D	2.58	129.50	124.68
11	L	305	U10	C20-C19-C21	2.57	119.60	115.27
8	M	402	BCL	C15-C13-C12	-2.57	98.61	112.13
8	3	101	BCL	OBB-CAB-CBB	-2.57	114.39	120.17
11	L	305	U10	C17-C18-C19	-2.57	121.48	127.66
10	H	301	PC1	O31-C31-C32	2.57	119.96	111.91
11	Y	501	U10	C22-C23-C24	-2.56	121.48	127.66
8	U	103	BCL	O2A-C1-C2	-2.56	101.90	108.64
8	0	102	BCL	C1C-NC-C4C	2.56	107.86	106.71
10	L	304	PC1	O31-C31-C32	2.56	119.94	111.91
11	M	404	U10	C20-C19-C21	2.56	119.58	115.27
8	3	101	BCL	CMD-C2D-C3D	2.55	129.45	124.68
8	O	101	BCL	CMD-C2D-C3D	2.55	129.45	124.68
8	U	103	BCL	C1C-NC-C4C	2.55	107.85	106.71
8	M	402	BCL	C2A-C1A-CHA	2.55	128.31	123.86
9	L	303	BPB	C11-C10-C8	-2.54	107.70	115.92
13	V	101	SPO	C40-C38-C39	2.54	120.22	114.60
8	J	102	BCL	C1C-NC-C4C	2.54	107.85	106.71
13	W	103	SPO	C16-C17-C19	2.54	122.83	118.94
8	L	307	BCL	OBB-CAB-CBB	-2.53	114.47	120.17
8	J	102	BCL	C2A-C1A-CHA	2.53	128.29	123.86
8	R	101	BCL	C2A-C1A-CHA	2.53	128.29	123.86
8	D	101	BCL	CMD-C2D-C3D	2.53	129.41	124.68
11	Y	501	U10	C10-C9-C11	2.52	119.51	115.27
8	J	102	BCL	CMD-C2D-C3D	2.52	129.40	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	306	PC1	O31-C31-C32	2.52	119.82	111.91
10	D	104	PC1	O31-C31-C32	2.52	119.81	111.91
8	A	101	BCL	CMD-C2D-C3D	2.51	129.38	124.68
8	9	101	BCL	OBB-CAB-CBB	-2.51	114.53	120.17
14	M	406	CDL	OA8-CA7-C31	2.51	119.77	111.91
9	M	403	BPB	CMB-C2B-C3B	2.51	129.37	124.68
11	L	305	U10	C10-C9-C11	2.51	119.48	115.27
14	M	406	CDL	OB8-CB7-C71	2.50	119.77	111.91
8	O	103	BCL	C1C-NC-C4C	2.50	107.83	106.71
13	3	104	SPO	C8-C7-C9	2.50	126.42	122.92
13	B	101	SPO	C36-C37-C38	-2.49	119.24	127.75
8	K	101	BCL	C1C-NC-C4C	2.49	107.82	106.71
9	L	303	BPB	CMD-C2D-C3D	2.49	129.33	124.68
13	N	102	SPO	C40-C38-C39	2.49	120.09	114.60
8	S	102	BCL	CMD-C2D-C3D	2.48	129.33	124.68
8	Q	101	BCL	OBB-CAB-CBB	-2.48	114.58	120.17
8	A	103	BCL	CMB-C2B-C3B	2.48	129.32	124.68
8	S	102	BCL	C6-C5-C3	2.48	119.96	113.45
8	O	103	BCL	CMD-C2D-C3D	2.48	129.32	124.68
8	C	101	BCL	C1-C2-C3	2.48	130.33	126.04
8	A	101	BCL	OBB-CAB-CBB	-2.47	114.60	120.17
8	U	103	BCL	C2A-C1A-CHA	2.47	128.18	123.86
8	A	103	BCL	CMD-C2D-C3D	2.47	129.30	124.68
8	1	102	BCL	CMD-C2D-C3D	2.47	129.29	124.68
8	F	103	BCL	CMD-C2D-C3D	2.46	129.28	124.68
8	A	101	BCL	C1C-NC-C4C	2.46	107.81	106.71
8	O	101	BCL	C1C-NC-C4C	2.46	107.81	106.71
8	C	101	BCL	O2A-C1-C2	-2.46	102.17	108.64
8	C	101	BCL	C4B-C3B-CAB	-2.46	122.38	127.13
8	O	101	BCL	OBB-CAB-CBB	-2.46	114.64	120.17
8	L	301	BCL	OBB-CAB-CBB	-2.45	114.64	120.17
13	M	405	SPO	C40-C38-C39	2.45	120.02	114.60
8	L	307	BCL	CMD-C2D-C3D	2.45	129.26	124.68
8	0	102	BCL	CMD-C2D-C3D	2.45	129.26	124.68
13	M	405	SPO	C36-C37-C38	-2.45	119.38	127.75
8	W	102	BCL	CMD-C2D-C3D	2.45	129.26	124.68
8	S	101	BCL	OBB-CAB-CBB	-2.45	114.66	120.17
8	I	101	BCL	C1C-NC-C4C	2.44	107.81	106.71
13	0	101	SPO	C25-C23-C22	-2.44	115.19	118.94
8	D	101	BCL	OBB-CAB-CBB	-2.44	114.67	120.17
8	0	102	BCL	C4A-NA-C1A	2.44	107.80	106.71
8	E	101	BCL	CMD-C2D-C3D	2.44	129.24	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	101	BCL	C2A-C1A-CHA	2.44	128.12	123.86
8	U	101	BCL	CMD-C2D-C3D	2.44	129.24	124.68
8	7	101	BCL	C4B-C3B-CAB	-2.44	122.42	127.13
8	S	102	BCL	C11-C10-C8	2.44	123.79	115.92
8	9	101	BCL	CMD-C2D-C3D	2.43	129.23	124.68
8	L	307	BCL	CAA-CBA-CGA	2.43	120.36	113.25
8	C	101	BCL	C17-C16-C15	2.43	124.40	113.24
8	3	103	BCL	CMD-C2D-C3D	2.43	129.22	124.68
8	1	101	BCL	CMD-C2D-C3D	2.43	129.22	124.68
8	E	101	BCL	C2A-C1A-CHA	2.42	128.10	123.86
8	1	101	BCL	OBB-CAB-CBB	-2.42	114.72	120.17
8	R	101	BCL	CMD-C2D-C3D	2.42	129.20	124.68
13	N	102	SPO	C14-C15-C16	-2.42	115.68	123.22
8	0	102	BCL	O2A-C1-C2	-2.41	102.29	108.64
8	I	101	BCL	CMD-C2D-C3D	2.41	129.19	124.68
8	N	101	BCL	CMD-C2D-C3D	2.41	129.19	124.68
8	1	102	BCL	CMB-C2B-C3B	2.41	129.19	124.68
8	Q	101	BCL	CMD-C2D-C3D	2.41	129.18	124.68
9	M	403	BPB	CMD-C2D-C3D	2.41	129.18	124.68
8	O	103	BCL	O2A-C1-C2	-2.40	102.31	108.64
11	L	305	U10	C27-C28-C29	-2.40	121.87	127.66
13	X	101	SPO	C10-C9-C7	-2.40	123.88	127.31
8	S	101	BCL	C1C-NC-C4C	2.40	107.78	106.71
8	J	102	BCL	O2A-C1-C2	-2.40	102.34	108.64
13	T	102	SPO	C31-C30-C28	2.40	120.86	112.98
13	N	102	SPO	C1-C4-C5	-2.39	106.71	113.06
8	8	101	BCL	C1C-NC-C4C	2.39	107.78	106.71
8	9	101	BCL	O2A-CGA-O1A	-2.39	117.56	123.59
11	Y	501	U10	C31-C29-C30	2.39	119.88	114.60
8	I	101	BCL	OBB-CAB-CBB	-2.39	114.80	120.17
11	L	308	U10	C31-C29-C30	2.38	119.87	114.60
8	R	101	BCL	C1C-NC-C4C	2.38	107.78	106.71
8	3	101	BCL	C1C-NC-C4C	2.38	107.78	106.71
8	F	101	BCL	OBB-CAB-CBB	-2.38	114.82	120.17
8	U	101	BCL	OBB-CAB-CBB	-2.36	114.85	120.17
8	7	101	BCL	C4A-NA-C1A	2.36	107.77	106.71
13	E	102	SPO	C15-C14-C12	-2.36	123.94	127.31
8	1	101	BCL	C1C-NC-C4C	2.35	107.76	106.71
8	K	101	BCL	CMD-C2D-C3D	2.35	129.07	124.68
8	F	103	BCL	C11-C10-C8	2.34	123.50	115.92
8	3	103	BCL	O2A-C1-C2	-2.34	102.48	108.64
13	J	101	SPO	C1-C4-C5	-2.34	106.86	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	103	BCL	C1C-NC-C4C	2.34	107.76	106.71
8	F	103	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
11	L	308	U10	C27-C28-C29	-2.34	119.77	127.75
8	L	307	BCL	C1C-NC-C4C	2.33	107.75	106.71
11	Y	501	U10	C27-C28-C29	-2.33	119.78	127.75
8	M	402	BCL	CMD-C2D-C3D	2.33	129.04	124.68
14	H	304	CDL	C57-C56-C55	2.33	131.10	113.42
8	L	301	BCL	CMD-C2D-C3D	2.33	129.03	124.68
8	A	103	BCL	C17-C16-C15	2.33	123.92	113.24
8	S	101	BCL	CMD-C2D-C3D	2.32	129.03	124.68
8	A	103	BCL	C4A-NA-C1A	2.32	107.75	106.71
8	K	101	BCL	OBB-CAB-CBB	-2.32	114.94	120.17
8	N	101	BCL	C1-O2A-CGA	2.32	122.53	116.44
10	A	102	PC1	C2-O21-C21	-2.32	112.08	117.79
8	W	102	BCL	OBB-CAB-CBB	-2.32	114.95	120.17
8	8	101	BCL	CMD-C2D-C3D	2.32	129.02	124.68
11	L	308	U10	C15-C14-C16	2.32	119.17	115.27
8	E	101	BCL	O2A-C1-C2	-2.31	102.56	108.64
8	9	101	BCL	C1C-NC-C4C	2.31	107.74	106.71
8	3	103	BCL	C2A-C1A-CHA	2.30	127.88	123.86
13	T	102	SPO	C25-C23-C22	-2.30	115.42	118.94
8	E	101	BCL	C4B-C3B-CAB	-2.30	122.69	127.13
8	3	103	BCL	C1C-NC-C4C	2.29	107.74	106.71
8	O	103	BCL	OBB-CAB-CBB	-2.29	115.02	120.17
8	F	101	BCL	CMD-C2D-C3D	2.28	128.95	124.68
13	3	104	SPO	C21-C20-C19	2.28	128.14	123.47
13	F	102	SPO	C11-C12-C14	2.27	122.43	118.94
8	W	102	BCL	C1C-NC-C4C	2.27	107.73	106.71
13	V	101	SPO	C3-C1-C4	-2.27	107.37	110.86
8	L	301	BCL	C4B-C3B-CAB	-2.27	122.75	127.13
9	M	403	BPB	O2D-CGD-CBD	2.26	113.86	111.00
8	3	103	BCL	C4B-C3B-CAB	-2.26	122.77	127.13
8	W	102	BCL	C4B-C3B-CAB	-2.26	122.77	127.13
13	U	104	SPO	C40-C38-C39	2.25	119.58	114.60
8	A	103	BCL	C4B-C3B-CAB	-2.25	122.78	127.13
8	F	101	BCL	C4B-C3B-CAB	-2.25	122.78	127.13
8	9	101	BCL	C4B-C3B-CAB	-2.24	122.79	127.13
13	V	101	SPO	C36-C35-C33	2.24	120.36	112.98
8	F	103	BCL	C1C-NC-C4C	2.24	107.71	106.71
8	0	102	BCL	C6-C7-C8	-2.24	108.68	115.92
10	A	104	PC1	C2-O21-C21	-2.24	112.28	117.79
10	H	302	PC1	C2-O21-C21	-2.23	112.29	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	305	U10	C1M-C1-C6	-2.23	120.75	124.40
8	R	101	BCL	C4B-C3B-CAB	-2.23	122.82	127.13
8	F	101	BCL	C1C-NC-C4C	2.23	107.71	106.71
8	1	101	BCL	C4B-C3B-CAB	-2.22	122.84	127.13
8	U	103	BCL	C1-O2A-CGA	2.22	122.26	116.44
8	U	101	BCL	C4B-C3B-CAB	-2.20	122.87	127.13
13	I	102	SPO	C2-C1-C4	-2.20	107.48	110.86
8	N	101	BCL	C4B-C3B-CAB	-2.20	122.88	127.13
11	M	404	U10	O5-C5-C6	-2.20	117.70	121.55
13	O	102	SPO	C15-C14-C12	-2.20	124.18	127.31
13	B	101	SPO	C16-C17-C19	2.19	122.30	118.94
8	L	302	BCL	CMD-C2D-C3D	2.19	128.77	124.68
13	V	101	SPO	C36-C37-C38	-2.19	120.28	127.75
9	L	303	BPB	O2D-CGD-CBD	2.19	113.76	111.00
8	S	102	BCL	O2A-C1-C2	-2.18	102.90	108.64
8	J	102	BCL	C4B-C3B-CAB	-2.18	122.92	127.13
13	3	104	SPO	C36-C37-C38	-2.18	120.30	127.75
8	8	101	BCL	CMB-C2B-C3B	2.17	128.75	124.68
8	N	101	BCL	C1C-NC-C4C	2.17	107.68	106.71
8	1	101	BCL	O2A-CGA-O1A	-2.17	118.12	123.59
13	T	102	SPO	C40-C38-C39	2.15	119.36	114.60
13	8	102	SPO	C40-C38-C39	2.15	119.36	114.60
13	I	102	SPO	C31-C32-C33	-2.15	122.48	127.66
8	E	101	BCL	C1C-NC-C4C	2.15	107.67	106.71
8	K	101	BCL	C4B-C3B-CAB	-2.15	122.98	127.13
8	N	101	BCL	C6-C5-C3	2.15	119.08	113.45
13	U	102	SPO	C1-C4-C5	-2.14	107.38	113.06
13	O	102	SPO	C36-C35-C33	2.14	120.02	112.98
8	M	402	BCL	CED-O2D-CGD	2.14	120.78	115.94
13	I	102	SPO	C10-C9-C7	-2.13	124.26	127.31
8	S	102	BCL	C1C-NC-C4C	2.13	107.66	106.71
14	M	406	CDL	CA6-CA4-CA3	-2.12	106.77	111.79
8	N	101	BCL	C17-C16-C15	2.12	122.98	113.24
8	R	101	BCL	OBB-CAB-CBB	-2.11	115.41	120.17
8	F	103	BCL	C4A-NA-C1A	2.11	107.65	106.71
8	J	102	BCL	OBB-CAB-CBB	-2.11	115.42	120.17
8	L	307	BCL	C11-C12-C13	-2.11	109.11	115.92
10	L	304	PC1	C2-O21-C21	-2.11	112.61	117.79
11	L	305	U10	C15-C14-C16	2.10	118.81	115.27
13	8	102	SPO	C36-C37-C38	-2.10	120.58	127.75
11	L	305	U10	C32-C33-C34	-2.09	120.61	127.75
10	L	306	PC1	C11-C12-N	-2.09	108.81	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	308	U10	C7-C8-C9	-2.08	123.33	126.79
13	E	102	SPO	C40-C38-C39	2.07	119.18	114.60
13	D	103	SPO	C40-C38-C39	2.07	119.18	114.60
8	1	102	BCL	C11-C10-C8	-2.07	109.23	115.92
8	D	101	BCL	C4B-C3B-CAB	-2.06	123.14	127.13
8	0	102	BCL	C5-C3-C2	-2.06	116.95	121.12
13	U	102	SPO	C31-C30-C28	2.05	119.73	112.98
8	S	102	BCL	OBB-CAB-CBB	-2.05	115.55	120.17
8	S	102	BCL	C4C-CHD-C1D	2.05	128.91	125.88
8	0	102	BCL	OBB-CAB-CBB	-2.05	115.57	120.17
11	M	404	U10	C41-C39-C40	2.04	119.11	114.60
8	L	302	BCL	OBB-CAB-CBB	-2.03	115.60	120.17
8	1	101	BCL	O2A-CGA-CBA	2.03	118.27	111.91
13	U	104	SPO	C3-C1-C4	-2.02	107.75	110.86
13	G	101	SPO	C18-C17-C19	2.02	125.75	122.92
8	M	402	BCL	C4B-C3B-CAB	-2.02	123.23	127.13
8	U	103	BCL	OBB-CAB-CBB	-2.02	115.63	120.17
10	H	302	PC1	C23-C22-C21	-2.02	106.29	113.62
9	M	403	BPB	OBB-CAB-CBB	-2.02	115.63	120.17
13	O	102	SPO	C40-C38-C39	2.01	119.05	114.60
8	7	101	BCL	OBB-CAB-CBB	-2.01	115.65	120.17
11	M	404	U10	C4M-O4-C4	2.01	123.58	116.47
13	O	104	SPO	C36-C35-C33	2.00	119.57	112.98
13	W	103	SPO	C3-C1-C4	-2.00	107.78	110.86

There are no chirality outliers.

All (790) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	307	BCL	O2A-C1-C2-C3
8	A	103	BCL	C1A-C2A-CAA-CBA
8	E	101	BCL	C1A-C2A-CAA-CBA
8	F	103	BCL	C1A-C2A-CAA-CBA
8	J	102	BCL	C1A-C2A-CAA-CBA
8	N	101	BCL	C6-C7-C8-C9
8	O	103	BCL	C1A-C2A-CAA-CBA
8	R	101	BCL	C1A-C2A-CAA-CBA
8	U	103	BCL	C1A-C2A-CAA-CBA
8	C	101	BCL	C1A-C2A-CAA-CBA
8	3	103	BCL	C1A-C2A-CAA-CBA
8	1	102	BCL	C2A-CAA-CBA-CGA
8	1	102	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	1	102	BCL	C4C-C3C-CAC-CBC
8	7	101	BCL	O2A-C1-C2-C3
8	9	101	BCL	C4C-C3C-CAC-CBC
9	L	303	BPB	C2C-C3C-CAC-CBC
9	L	303	BPB	C4C-C3C-CAC-CBC
9	M	403	BPB	C2-C3-C5-C6
9	M	403	BPB	C4-C3-C5-C6
9	M	403	BPB	C2C-C3C-CAC-CBC
9	M	403	BPB	C4C-C3C-CAC-CBC
10	L	304	PC1	C11-O13-P-O12
10	L	304	PC1	C11-O13-P-O14
10	L	304	PC1	C1-O11-P-O14
10	L	306	PC1	C11-O13-P-O12
10	L	306	PC1	C11-O13-P-O14
10	L	306	PC1	C11-O13-P-O11
10	H	303	PC1	O22-C21-O21-C2
10	A	104	PC1	C11-O13-P-O12
10	A	104	PC1	C11-O13-P-O11
10	A	104	PC1	C1-O11-P-O14
10	A	104	PC1	O13-C11-C12-N
10	D	104	PC1	O13-C11-C12-N
10	W	101	PC1	O22-C21-O21-C2
10	W	101	PC1	C22-C21-O21-C2
11	L	305	U10	C12-C13-C14-C15
11	L	305	U10	C12-C13-C14-C16
11	L	305	U10	C24-C26-C27-C28
11	L	308	U10	C23-C24-C26-C27
11	L	308	U10	C25-C24-C26-C27
11	L	308	U10	C24-C26-C27-C28
11	M	404	U10	C34-C36-C37-C38
13	M	405	SPO	O1-C1-C4-C5
13	M	405	SPO	C2-C1-C4-C5
13	M	405	SPO	C3-C1-C4-C5
13	M	405	SPO	C5-C6-C7-C8
13	M	405	SPO	C5-C6-C7-C9
13	M	405	SPO	C10-C11-C12-C13
13	M	405	SPO	C10-C11-C12-C14
13	B	101	SPO	C10-C11-C12-C13
13	B	101	SPO	C10-C11-C12-C14
13	B	101	SPO	C15-C16-C17-C18
13	B	101	SPO	C15-C16-C17-C19
13	B	101	SPO	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
13	B	101	SPO	C33-C35-C36-C37
13	D	102	SPO	C5-C6-C7-C8
13	D	102	SPO	C5-C6-C7-C9
13	D	102	SPO	C28-C30-C31-C32
13	D	103	SPO	C5-C6-C7-C8
13	D	103	SPO	C5-C6-C7-C9
13	D	103	SPO	C11-C10-C9-C7
13	D	103	SPO	C12-C14-C15-C16
13	D	103	SPO	C15-C16-C17-C18
13	D	103	SPO	C15-C16-C17-C19
13	E	102	SPO	O1-C1-C4-C5
13	E	102	SPO	C2-C1-C4-C5
13	E	102	SPO	C3-C1-C4-C5
13	E	102	SPO	C10-C11-C12-C13
13	E	102	SPO	C10-C11-C12-C14
13	F	102	SPO	C15-C16-C17-C18
13	G	101	SPO	C2-C1-C4-C5
13	G	101	SPO	C3-C1-C4-C5
13	G	101	SPO	C15-C16-C17-C18
13	G	101	SPO	C15-C16-C17-C19
13	G	101	SPO	C22-C23-C25-C26
13	G	101	SPO	C25-C26-C27-C28
13	G	101	SPO	C28-C30-C31-C32
13	G	101	SPO	C32-C33-C35-C36
13	G	101	SPO	C34-C33-C35-C36
13	I	102	SPO	O1-C1-C4-C5
13	I	102	SPO	C2-C1-C4-C5
13	I	102	SPO	C3-C1-C4-C5
13	I	102	SPO	C10-C11-C12-C13
13	I	102	SPO	C10-C11-C12-C14
13	I	102	SPO	C15-C16-C17-C18
13	I	102	SPO	C15-C16-C17-C19
13	I	102	SPO	C22-C23-C25-C26
13	I	102	SPO	C24-C23-C25-C26
13	I	102	SPO	C27-C28-C30-C31
13	I	102	SPO	C29-C28-C30-C31
13	J	101	SPO	C10-C11-C12-C13
13	J	101	SPO	C10-C11-C12-C14
13	J	101	SPO	C26-C27-C28-C29
13	J	103	SPO	O1-C1-C4-C5
13	J	103	SPO	C2-C1-C4-C5
13	J	103	SPO	C3-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
13	J	103	SPO	C12-C14-C15-C16
13	J	103	SPO	C15-C16-C17-C18
13	J	103	SPO	C22-C23-C25-C26
13	J	103	SPO	C24-C23-C25-C26
13	J	103	SPO	C25-C26-C27-C28
13	J	103	SPO	C32-C33-C35-C36
13	J	103	SPO	C33-C35-C36-C37
13	N	102	SPO	C5-C6-C7-C8
13	N	102	SPO	C15-C16-C17-C18
13	N	102	SPO	C15-C16-C17-C19
13	N	102	SPO	C27-C28-C30-C31
13	N	102	SPO	C31-C32-C33-C35
13	O	102	SPO	C2-C1-C4-C5
13	O	102	SPO	C3-C1-C4-C5
13	O	102	SPO	C5-C6-C7-C8
13	O	102	SPO	C5-C6-C7-C9
13	O	102	SPO	C10-C11-C12-C13
13	O	102	SPO	C10-C11-C12-C14
13	O	102	SPO	C22-C23-C25-C26
13	O	102	SPO	C24-C23-C25-C26
13	O	102	SPO	C33-C35-C36-C37
13	O	104	SPO	C3-C1-O1-CM1
13	O	104	SPO	C5-C6-C7-C8
13	O	104	SPO	C5-C6-C7-C9
13	O	104	SPO	C15-C16-C17-C18
13	O	104	SPO	C15-C16-C17-C19
13	O	104	SPO	C28-C30-C31-C32
13	O	104	SPO	C32-C33-C35-C36
13	O	104	SPO	C33-C35-C36-C37
13	P	101	SPO	C1-C4-C5-C6
13	P	101	SPO	C10-C11-C12-C13
13	P	101	SPO	C10-C11-C12-C14
13	P	101	SPO	C15-C16-C17-C18
13	P	101	SPO	C15-C16-C17-C19
13	T	102	SPO	C4-C1-O1-CM1
13	T	102	SPO	C33-C35-C36-C37
13	U	102	SPO	O1-C1-C4-C5
13	U	102	SPO	C2-C1-C4-C5
13	U	102	SPO	C3-C1-C4-C5
13	U	102	SPO	C12-C14-C15-C16
13	U	102	SPO	C20-C21-C22-C23
13	U	102	SPO	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
13	U	102	SPO	C24-C23-C25-C26
13	U	102	SPO	C29-C28-C30-C31
13	U	104	SPO	C4-C1-O1-CM1
13	U	104	SPO	C2-C1-C4-C5
13	U	104	SPO	C3-C1-C4-C5
13	U	104	SPO	C5-C6-C7-C8
13	U	104	SPO	C5-C6-C7-C9
13	U	104	SPO	C33-C35-C36-C37
13	V	101	SPO	C1-C4-C5-C6
13	V	101	SPO	C5-C6-C7-C8
13	V	101	SPO	C5-C6-C7-C9
13	V	101	SPO	C10-C11-C12-C13
13	V	101	SPO	C10-C11-C12-C14
13	V	101	SPO	C32-C33-C35-C36
13	V	101	SPO	C34-C33-C35-C36
13	W	103	SPO	C2-C1-C4-C5
13	W	103	SPO	C3-C1-C4-C5
13	W	103	SPO	C15-C16-C17-C18
13	W	103	SPO	C22-C23-C25-C26
13	W	103	SPO	C24-C23-C25-C26
13	W	103	SPO	C26-C27-C28-C29
13	W	103	SPO	C32-C33-C35-C36
13	W	103	SPO	C34-C33-C35-C36
13	3	102	SPO	C15-C16-C17-C18
13	3	102	SPO	C33-C35-C36-C37
13	3	104	SPO	C2-C1-C4-C5
13	3	104	SPO	C1-C4-C5-C6
13	3	104	SPO	C5-C6-C7-C8
13	3	104	SPO	C32-C33-C35-C36
13	3	104	SPO	C33-C35-C36-C37
13	8	102	SPO	C2-C1-C4-C5
13	8	102	SPO	C3-C1-C4-C5
13	8	102	SPO	C1-C4-C5-C6
13	8	102	SPO	C12-C14-C15-C16
13	8	102	SPO	C15-C16-C17-C18
13	8	102	SPO	C15-C16-C17-C19
13	8	102	SPO	C22-C23-C25-C26
13	8	102	SPO	C24-C23-C25-C26
13	8	102	SPO	C28-C30-C31-C32
13	9	102	SPO	C15-C16-C17-C18
13	9	102	SPO	C15-C16-C17-C19
13	0	101	SPO	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	0	101	SPO	C5-C6-C7-C9
13	0	101	SPO	C10-C11-C12-C13
13	0	101	SPO	C10-C11-C12-C14
13	0	101	SPO	C15-C16-C17-C18
13	0	101	SPO	C15-C16-C17-C19
13	0	101	SPO	C33-C35-C36-C37
13	X	101	SPO	C2-C1-C4-C5
13	X	101	SPO	C3-C1-C4-C5
13	X	101	SPO	C10-C11-C12-C13
13	X	101	SPO	C10-C11-C12-C14
13	X	101	SPO	C15-C16-C17-C18
13	X	101	SPO	C15-C16-C17-C19
13	X	101	SPO	C28-C30-C31-C32
13	X	101	SPO	C33-C35-C36-C37
14	M	406	CDL	CA2-C1-CB2-OB2
14	M	406	CDL	CA3-OA5-PA1-OA3
14	M	406	CDL	OA7-CA5-OA6-CA4
14	M	406	CDL	C11-CA5-OA6-CA4
14	M	406	CDL	CB3-OB5-PB2-OB3
14	M	406	CDL	OB9-CB7-OB8-CB6
14	M	406	CDL	C71-CB7-OB8-CB6
14	H	304	CDL	CB2-C1-CA2-OA2
14	H	304	CDL	CA3-OA5-PA1-OA2
14	H	304	CDL	C11-CA5-OA6-CA4
14	H	304	CDL	C1-CB2-OB2-PB2
14	H	304	CDL	OA9-CA7-OA8-CA6
14	H	304	CDL	C31-CA7-OA8-CA6
14	H	304	CDL	OA7-CA5-OA6-CA4
13	N	102	SPO	C29-C28-C30-C31
13	M	405	SPO	C31-C32-C33-C35
13	E	102	SPO	C12-C14-C15-C16
13	G	101	SPO	C12-C14-C15-C16
13	N	102	SPO	C11-C10-C9-C7
13	N	102	SPO	C12-C14-C15-C16
13	U	104	SPO	C12-C14-C15-C16
13	8	102	SPO	C20-C21-C22-C23
13	8	102	SPO	C25-C26-C27-C28
13	9	102	SPO	C25-C26-C27-C28
13	X	101	SPO	C25-C26-C27-C28
14	H	304	CDL	O1-C1-CA2-OA2
14	H	304	CDL	C33-C34-C35-C36
14	M	406	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	1	102	BCL	C4-C3-C5-C6
13	E	102	SPO	C29-C28-C30-C31
13	T	102	SPO	C29-C28-C30-C31
13	9	102	SPO	C34-C33-C35-C36
8	1	102	BCL	C2-C3-C5-C6
13	E	102	SPO	C27-C28-C30-C31
13	T	102	SPO	C27-C28-C30-C31
13	U	102	SPO	C27-C28-C30-C31
13	V	101	SPO	C27-C28-C30-C31
13	9	102	SPO	C32-C33-C35-C36
10	W	101	PC1	C24-C25-C26-C27
11	L	305	U10	C9-C11-C12-C13
11	L	305	U10	C14-C16-C17-C18
11	L	308	U10	C14-C16-C17-C18
13	M	405	SPO	C33-C35-C36-C37
13	D	102	SPO	C33-C35-C36-C37
13	D	103	SPO	C28-C30-C31-C32
13	D	103	SPO	C33-C35-C36-C37
13	E	102	SPO	C33-C35-C36-C37
13	F	102	SPO	C28-C30-C31-C32
13	F	102	SPO	C33-C35-C36-C37
13	G	101	SPO	C33-C35-C36-C37
13	I	102	SPO	C33-C35-C36-C37
13	J	101	SPO	C28-C30-C31-C32
13	O	102	SPO	C28-C30-C31-C32
13	P	101	SPO	C33-C35-C36-C37
13	W	103	SPO	C28-C30-C31-C32
13	W	103	SPO	C33-C35-C36-C37
13	8	102	SPO	C33-C35-C36-C37
13	9	102	SPO	C28-C30-C31-C32
10	A	102	PC1	C11-C12-N-C13
10	A	104	PC1	C32-C31-O31-C3
10	D	104	PC1	C32-C31-O31-C3
14	M	406	CDL	C31-CA7-OA8-CA6
10	D	104	PC1	C23-C24-C25-C26
13	J	103	SPO	C11-C10-C9-C7
13	N	102	SPO	C20-C21-C22-C23
10	H	301	PC1	C25-C26-C27-C28
14	M	406	CDL	O1-C1-CB2-OB2
10	A	104	PC1	O32-C31-O31-C3
8	L	307	BCL	C6-C7-C8-C9
8	E	101	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
8	U	103	BCL	C6-C7-C8-C9
8	7	101	BCL	C6-C7-C8-C9
13	M	405	SPO	C15-C16-C17-C18
13	B	101	SPO	C24-C23-C25-C26
13	D	102	SPO	C24-C23-C25-C26
13	E	102	SPO	C5-C6-C7-C8
13	F	102	SPO	C10-C11-C12-C13
13	F	102	SPO	C24-C23-C25-C26
13	G	101	SPO	C24-C23-C25-C26
13	J	101	SPO	C24-C23-C25-C26
13	J	103	SPO	C10-C11-C12-C13
13	N	102	SPO	C24-C23-C25-C26
13	P	101	SPO	C5-C6-C7-C8
13	P	101	SPO	C24-C23-C25-C26
13	T	101	SPO	C24-C23-C25-C26
13	T	102	SPO	C5-C6-C7-C8
13	T	102	SPO	C10-C11-C12-C13
13	U	102	SPO	C10-C11-C12-C13
13	U	102	SPO	C15-C16-C17-C18
13	U	104	SPO	C10-C11-C12-C13
13	U	104	SPO	C15-C16-C17-C18
13	W	103	SPO	C5-C6-C7-C8
13	3	104	SPO	C24-C23-C25-C26
13	8	102	SPO	C10-C11-C12-C13
13	9	102	SPO	C10-C11-C12-C13
13	9	102	SPO	C24-C23-C25-C26
13	X	101	SPO	C24-C23-C25-C26
13	M	405	SPO	C15-C16-C17-C19
13	B	101	SPO	C22-C23-C25-C26
13	D	102	SPO	C22-C23-C25-C26
13	E	102	SPO	C5-C6-C7-C9
13	F	102	SPO	C10-C11-C12-C14
13	F	102	SPO	C22-C23-C25-C26
13	J	103	SPO	C10-C11-C12-C14
13	N	102	SPO	C10-C11-C12-C14
13	N	102	SPO	C22-C23-C25-C26
13	O	104	SPO	C22-C23-C25-C26
13	P	101	SPO	C5-C6-C7-C9
13	P	101	SPO	C22-C23-C25-C26
13	T	101	SPO	C22-C23-C25-C26
13	T	102	SPO	C10-C11-C12-C14
13	U	102	SPO	C10-C11-C12-C14

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Mol	Chain	Res	Type	Atoms
13	U	102	SPO	C15-C16-C17-C19
13	U	104	SPO	C10-C11-C12-C14
13	U	104	SPO	C15-C16-C17-C19
13	W	103	SPO	C5-C6-C7-C9
13	W	103	SPO	C10-C11-C12-C14
13	3	104	SPO	C5-C6-C7-C9
13	3	104	SPO	C22-C23-C25-C26
13	8	102	SPO	C10-C11-C12-C14
13	9	102	SPO	C10-C11-C12-C14
13	9	102	SPO	C22-C23-C25-C26
13	0	101	SPO	C22-C23-C25-C26
13	X	101	SPO	C22-C23-C25-C26
8	W	102	BCL	C10-C11-C12-C13
11	L	305	U10	C7-C8-C9-C10
11	Y	501	U10	C7-C8-C9-C10
14	H	304	CDL	C75-C76-C77-C78
10	A	102	PC1	C11-C12-N-C14
10	H	301	PC1	C21-C22-C23-C24
13	T	101	SPO	C20-C21-C22-C23
13	U	102	SPO	C17-C19-C20-C21
13	9	102	SPO	C20-C21-C22-C23
8	N	101	BCL	C10-C11-C12-C13
14	M	406	CDL	C82-C83-C84-C85
10	D	104	PC1	O32-C31-O31-C3
13	B	101	SPO	C28-C30-C31-C32
13	N	102	SPO	C28-C30-C31-C32
13	N	102	SPO	C33-C35-C36-C37
13	P	101	SPO	C28-C30-C31-C32
13	T	101	SPO	C28-C30-C31-C32
13	U	102	SPO	C33-C35-C36-C37
13	U	104	SPO	C28-C30-C31-C32
8	7	101	BCL	C5-C6-C7-C8
14	M	406	CDL	OA9-CA7-OA8-CA6
10	L	304	PC1	C32-C33-C34-C35
8	S	102	BCL	C13-C15-C16-C17
10	L	304	PC1	C11-O13-P-O11
10	L	304	PC1	C1-O11-P-O13
10	A	102	PC1	C11-O13-P-O11
10	A	104	PC1	C1-O11-P-O13
14	M	406	CDL	CA3-OA5-PA1-OA2
14	M	406	CDL	CB3-OB5-PB2-OB2
10	A	102	PC1	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
14	H	304	CDL	C71-CB7-OB8-CB6
8	1	101	BCL	C4-C3-C5-C6
13	O	104	SPO	C34-C33-C35-C36
13	9	102	SPO	C11-C10-C9-C7
8	F	101	BCL	C10-C11-C12-C13
8	1	101	BCL	C5-C6-C7-C8
14	H	304	CDL	C34-C35-C36-C37
14	H	304	CDL	C37-C38-C39-C40
10	L	304	PC1	C23-C24-C25-C26
10	H	301	PC1	C23-C24-C25-C26
14	M	406	CDL	C60-C61-C62-C63
8	F	103	BCL	C5-C6-C7-C8
8	O	103	BCL	C13-C15-C16-C17
14	H	304	CDL	C82-C83-C84-C85
14	M	406	CDL	C43-C44-C45-C46
10	D	104	PC1	C22-C23-C24-C25
14	M	406	CDL	C73-C74-C75-C76
14	M	406	CDL	C20-C21-C22-C23
8	S	102	BCL	C4-C3-C5-C6
11	L	305	U10	C15-C14-C16-C17
14	H	304	CDL	C41-C42-C43-C44
8	1	101	BCL	C2-C3-C5-C6
8	O	101	BCL	C6-C7-C8-C9
10	H	301	PC1	C26-C27-C28-C29
13	G	101	SPO	C10-C11-C12-C13
13	N	102	SPO	C10-C11-C12-C13
13	O	104	SPO	C24-C23-C25-C26
13	T	102	SPO	C24-C23-C25-C26
13	W	103	SPO	C10-C11-C12-C13
13	8	102	SPO	C5-C6-C7-C8
13	0	101	SPO	C24-C23-C25-C26
10	H	301	PC1	C22-C23-C24-C25
13	F	102	SPO	C15-C16-C17-C19
13	G	101	SPO	C10-C11-C12-C14
13	J	101	SPO	C22-C23-C25-C26
13	T	102	SPO	C5-C6-C7-C9
13	T	102	SPO	C22-C23-C25-C26
13	8	102	SPO	C5-C6-C7-C9
10	A	102	PC1	C34-C35-C36-C37
14	M	406	CDL	C71-C72-C73-C74
13	T	102	SPO	C28-C30-C31-C32
14	M	406	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
14	M	406	CDL	C38-C39-C40-C41
14	H	304	CDL	C73-C74-C75-C76
10	W	101	PC1	C32-C31-O31-C3
8	A	103	BCL	C3A-C2A-CAA-CBA
8	E	101	BCL	C3A-C2A-CAA-CBA
8	F	103	BCL	C3A-C2A-CAA-CBA
8	J	102	BCL	C3A-C2A-CAA-CBA
8	N	101	BCL	C3A-C2A-CAA-CBA
8	O	103	BCL	C3A-C2A-CAA-CBA
8	R	101	BCL	C3A-C2A-CAA-CBA
8	U	103	BCL	C3A-C2A-CAA-CBA
8	C	101	BCL	C3A-C2A-CAA-CBA
8	3	103	BCL	C3A-C2A-CAA-CBA
13	T	102	SPO	C11-C10-C9-C7
14	M	406	CDL	C35-C36-C37-C38
14	M	406	CDL	C80-C81-C82-C83
14	H	304	CDL	C72-C73-C74-C75
14	H	304	CDL	C40-C41-C42-C43
14	H	304	CDL	OB9-CB7-OB8-CB6
8	C	101	BCL	C4-C3-C5-C6
13	J	103	SPO	C34-C33-C35-C36
8	O	101	BCL	C2-C3-C5-C6
8	C	101	BCL	C2-C3-C5-C6
9	L	303	BPB	C2-C3-C5-C6
11	L	305	U10	C13-C14-C16-C17
13	U	104	SPO	C32-C33-C35-C36
13	0	101	SPO	C35-C36-C37-C38
10	W	101	PC1	O32-C31-O31-C3
10	A	102	PC1	C11-C12-N-C15
10	A	104	PC1	C22-C23-C24-C25
8	L	307	BCL	C8-C10-C11-C12
8	O	101	BCL	C4-C3-C5-C6
8	S	101	BCL	C4-C3-C5-C6
9	L	303	BPB	C4-C3-C5-C6
8	O	101	BCL	C6-C7-C8-C10
8	S	101	BCL	C2-C3-C5-C6
8	S	102	BCL	C2-C3-C5-C6
8	U	103	BCL	C6-C7-C8-C10
13	B	101	SPO	C25-C26-C27-C28
13	P	101	SPO	C12-C14-C15-C16
13	W	103	SPO	C11-C10-C9-C7
13	X	101	SPO	C11-C10-C9-C7

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Mol	Chain	Res	Type	Atoms
14	M	406	CDL	C17-C18-C19-C20
14	M	406	CDL	C76-C77-C78-C79
14	H	304	CDL	CB5-C51-C52-C53
10	H	302	PC1	C22-C21-O21-C2
10	A	104	PC1	C22-C21-O21-C2
13	J	103	SPO	C14-C15-C16-C17
10	H	301	PC1	O21-C2-C3-O31
14	M	406	CDL	C81-C82-C83-C84
13	N	102	SPO	C32-C33-C35-C36
13	8	102	SPO	C27-C28-C30-C31
13	0	101	SPO	C27-C28-C30-C31
10	L	304	PC1	C25-C26-C27-C28
14	H	304	CDL	C71-C72-C73-C74
13	V	101	SPO	C24-C23-C25-C26
13	V	101	SPO	C22-C23-C25-C26
13	W	103	SPO	C15-C16-C17-C19
13	3	102	SPO	C15-C16-C17-C19
8	N	101	BCL	C1A-C2A-CAA-CBA
10	H	302	PC1	O22-C21-O21-C2
10	A	104	PC1	O22-C21-O21-C2
13	F	102	SPO	C11-C10-C9-C7
10	H	301	PC1	C11-O13-P-O11
10	W	101	PC1	C11-O13-P-O11
14	M	406	CDL	OB5-CB3-CB4-CB6
14	M	406	CDL	C34-C35-C36-C37
13	W	103	SPO	C1-C4-C5-C6
14	M	406	CDL	CA7-C31-C32-C33
13	8	102	SPO	C29-C28-C30-C31
10	H	302	PC1	C29-C2A-C2B-C2C
10	L	306	PC1	C37-C38-C39-C3A
10	H	301	PC1	C1-C2-C3-O31
14	H	304	CDL	C54-C55-C56-C57
14	M	406	CDL	C57-C58-C59-C60
10	H	302	PC1	C21-C22-C23-C24
14	H	304	CDL	C44-C45-C46-C47
11	Y	501	U10	C20-C19-C21-C22
13	3	104	SPO	C34-C33-C35-C36
14	H	304	CDL	CA3-CA4-OA6-CA5
14	M	406	CDL	C61-C62-C63-C64
10	A	102	PC1	O11-C1-C2-O21
13	O	104	SPO	C2-C1-O1-CM1
13	T	102	SPO	C2-C1-O1-CM1

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Mol	Chain	Res	Type	Atoms
13	T	102	SPO	C3-C1-O1-CM1
13	U	104	SPO	C2-C1-O1-CM1
10	L	306	PC1	O21-C2-C3-O31
13	F	102	SPO	C2-C1-C4-C5
13	J	101	SPO	C2-C1-C4-C5
13	J	101	SPO	C3-C1-C4-C5
13	N	102	SPO	C2-C1-C4-C5
13	N	102	SPO	C3-C1-C4-C5
13	V	101	SPO	C2-C1-C4-C5
13	V	101	SPO	C3-C1-C4-C5
13	3	104	SPO	C3-C1-C4-C5
13	9	102	SPO	C2-C1-C4-C5
11	L	305	U10	C30-C29-C31-C32
8	9	101	BCL	C11-C10-C8-C7
11	L	305	U10	C28-C29-C31-C32
8	A	103	BCL	C11-C12-C13-C14
13	G	101	SPO	O1-C1-C4-C5
13	O	102	SPO	O1-C1-C4-C5
13	8	102	SPO	O1-C1-C4-C5
13	J	101	SPO	C5-C6-C7-C8
14	M	406	CDL	C24-C25-C26-C27
13	E	102	SPO	C15-C16-C17-C19
13	J	101	SPO	C5-C6-C7-C9
14	M	406	CDL	C36-C37-C38-C39
10	A	102	PC1	O11-C1-C2-C3
11	M	404	U10	C14-C16-C17-C18
8	7	101	BCL	C4-C3-C5-C6
11	L	305	U10	C20-C19-C21-C22
11	M	404	U10	C30-C29-C31-C32
11	M	404	U10	C28-C29-C31-C32
14	M	406	CDL	CB5-C51-C52-C53
14	M	406	CDL	C54-C55-C56-C57
14	M	406	CDL	C1-CA2-OA2-PA1
13	T	101	SPO	C25-C26-C27-C28
13	U	102	SPO	C11-C10-C9-C7
14	H	304	CDL	C12-C13-C14-C15
10	H	302	PC1	C32-C31-O31-C3
14	M	406	CDL	C84-C85-C86-C87
8	0	102	BCL	C4-C3-C5-C6
13	M	405	SPO	C34-C33-C35-C36
13	0	101	SPO	C29-C28-C30-C31
11	L	305	U10	C18-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
14	M	406	CDL	C51-C52-C53-C54
14	H	304	CDL	C38-C39-C40-C41
14	M	406	CDL	OB5-CB3-CB4-OB6
10	L	306	PC1	C32-C31-O31-C3
11	L	305	U10	C29-C31-C32-C33
13	V	101	SPO	C33-C35-C36-C37
8	O	101	BCL	C5-C6-C7-C8
10	A	104	PC1	C2-C1-O11-P
10	D	104	PC1	C11-C12-N-C15
14	M	406	CDL	C37-C38-C39-C40
13	J	103	SPO	C15-C16-C17-C19
13	N	102	SPO	C5-C6-C7-C9
10	H	302	PC1	C24-C25-C26-C27
8	U	101	BCL	C10-C11-C12-C13
10	H	301	PC1	O11-C1-C2-C3
8	E	101	BCL	C12-C13-C15-C16
8	N	101	BCL	C6-C7-C8-C10
8	N	101	BCL	C11-C12-C13-C15
11	Y	501	U10	C18-C19-C21-C22
13	F	102	SPO	C25-C26-C27-C28
13	I	102	SPO	C11-C10-C9-C7
13	N	102	SPO	C25-C26-C27-C28
13	T	102	SPO	C25-C26-C27-C28
13	W	103	SPO	C20-C21-C22-C23
13	0	101	SPO	C11-C10-C9-C7
10	L	304	PC1	C22-C21-O21-C2
13	N	102	SPO	C21-C22-C23-C24
8	M	402	BCL	CAD-CBD-CGD-O2D
9	L	303	BPB	CAD-CBD-CGD-O2D
9	M	403	BPB	CAD-CBD-CGD-O2D
13	M	405	SPO	C26-C27-C28-C29
13	J	103	SPO	C26-C27-C28-C29
13	T	101	SPO	C26-C27-C28-C29
13	9	102	SPO	C26-C27-C28-C29
11	L	305	U10	C5-C4-O4-C4M
11	Y	501	U10	C5-C4-O4-C4M
10	H	301	PC1	O11-C1-C2-O21
14	M	406	CDL	OA5-CA3-CA4-OA6
14	H	304	CDL	C52-C53-C54-C55
10	H	302	PC1	O32-C31-O31-C3
10	H	302	PC1	C2A-C2B-C2C-C2D
10	H	302	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
10	L	306	PC1	O32-C31-O31-C3
13	U	104	SPO	C27-C28-C30-C31
10	L	304	PC1	O22-C21-O21-C2
8	N	101	BCL	C11-C12-C13-C14
13	E	102	SPO	C15-C16-C17-C18
13	X	101	SPO	C5-C6-C7-C8
13	D	103	SPO	C25-C26-C27-C28
14	M	406	CDL	CA2-OA2-PA1-OA5
14	M	406	CDL	CB2-OB2-PB2-OB5
10	H	301	PC1	C29-C2A-C2B-C2C
13	U	104	SPO	C29-C28-C30-C31
14	M	406	CDL	C72-C73-C74-C75
10	L	304	PC1	C1-O11-P-O12
10	H	301	PC1	C11-O13-P-O12
10	A	102	PC1	C11-O13-P-O14
10	A	102	PC1	C1-O11-P-O12
10	A	104	PC1	C11-O13-P-O14
10	D	104	PC1	C11-C12-N-C14
10	W	101	PC1	C11-O13-P-O12
11	L	308	U10	C6-C7-C8-C9
14	M	406	CDL	CA3-OA5-PA1-OA4
14	M	406	CDL	OA5-CA3-CA4-CA6
14	H	304	CDL	OA5-CA3-CA4-CA6
14	H	304	CDL	OB7-CB5-OB6-CB4
8	F	101	BCL	C6-C7-C8-C10
8	U	101	BCL	C6-C7-C8-C10
8	0	102	BCL	C2-C3-C5-C6
14	H	304	CDL	OA5-CA3-CA4-OA6
13	W	103	SPO	C12-C14-C15-C16
14	H	304	CDL	C31-C32-C33-C34
10	H	303	PC1	C11-C12-N-C15
10	L	306	PC1	O13-C11-C12-N
10	L	306	PC1	C1-C2-C3-O31
10	H	301	PC1	O13-C11-C12-N
10	H	302	PC1	O13-C11-C12-N
10	H	303	PC1	O13-C11-C12-N
10	W	101	PC1	O13-C11-C12-N
14	M	406	CDL	C83-C84-C85-C86
14	M	406	CDL	C32-C33-C34-C35
10	L	306	PC1	C36-C37-C38-C39
14	M	406	CDL	C15-C16-C17-C18
8	7	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	M	402	BCL	C14-C13-C15-C16
8	F	101	BCL	C6-C7-C8-C9
8	9	101	BCL	C11-C10-C8-C9
13	J	103	SPO	C28-C30-C31-C32
13	3	102	SPO	C28-C30-C31-C32
13	T	102	SPO	C14-C15-C16-C17
13	3	104	SPO	C14-C15-C16-C17
13	8	102	SPO	C23-C25-C26-C27
13	M	405	SPO	C11-C10-C9-C7
13	J	101	SPO	C25-C26-C27-C28
13	W	103	SPO	C25-C26-C27-C28
11	L	308	U10	C5-C4-O4-C4M
10	D	104	PC1	C24-C25-C26-C27
10	W	101	PC1	C33-C34-C35-C36
10	H	303	PC1	C11-C12-N-C14
14	H	304	CDL	C83-C84-C85-C86
13	O	102	SPO	C32-C33-C35-C36
10	D	104	PC1	C32-C33-C34-C35
14	H	304	CDL	C51-CB5-OB6-CB4
13	U	104	SPO	C3-C1-O1-CM1
13	8	102	SPO	C3-C1-O1-CM1
14	H	304	CDL	CA2-OA2-PA1-OA5
13	T	101	SPO	C2-C1-C4-C5
10	H	302	PC1	C1-C2-C3-O31
8	7	101	BCL	C6-C7-C8-C10
8	U	101	BCL	C6-C7-C8-C9
8	U	103	BCL	C11-C12-C13-C14
13	N	102	SPO	O1-C1-C4-C5
13	P	101	SPO	O1-C1-C4-C5
13	X	101	SPO	O1-C1-C4-C5
8	U	103	BCL	C4-C3-C5-C6
11	Y	501	U10	C7-C8-C9-C11
10	D	104	PC1	C11-C12-N-C13
13	B	101	SPO	C20-C21-C22-C23
13	I	102	SPO	C25-C26-C27-C28
13	O	104	SPO	C25-C26-C27-C28
13	U	104	SPO	C25-C26-C27-C28
8	U	103	BCL	C2-C3-C5-C6
10	H	301	PC1	C35-C36-C37-C38
8	9	101	BCL	C10-C11-C12-C13
8	N	101	BCL	C2-C1-O2A-CGA
14	H	304	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
8	N	101	BCL	C11-C10-C8-C9
8	S	101	BCL	C14-C13-C15-C16
8	S	102	BCL	C6-C7-C8-C9
10	A	104	PC1	C1-C2-C3-O31
13	T	102	SPO	C21-C22-C23-C24
13	3	104	SPO	C8-C7-C9-C10
13	3	104	SPO	C13-C12-C14-C15
13	3	104	SPO	C18-C17-C19-C20
13	8	102	SPO	C21-C22-C23-C24
11	L	305	U10	C7-C8-C9-C11
9	L	303	BPB	O2A-C1-C2-C3
10	H	303	PC1	C11-C12-N-C13
10	W	101	PC1	C31-C32-C33-C34
13	J	101	SPO	C11-C10-C9-C7
8	C	101	BCL	C10-C11-C12-C13
11	L	305	U10	C3-C4-O4-C4M
10	L	306	PC1	C32-C33-C34-C35
10	H	301	PC1	C2-C1-O11-P
14	M	406	CDL	CB7-C71-C72-C73
11	Y	501	U10	C25-C24-C26-C27
13	3	104	SPO	C29-C28-C30-C31
10	D	104	PC1	C28-C29-C2A-C2B
13	T	102	SPO	C21-C22-C23-C25
13	3	104	SPO	C6-C7-C9-C10
13	3	104	SPO	C11-C12-C14-C15
13	3	104	SPO	C16-C17-C19-C20
10	H	302	PC1	O21-C2-C3-O31
10	W	101	PC1	O21-C2-C3-O31
13	B	101	SPO	C17-C19-C20-C21
13	I	102	SPO	C20-C21-C22-C23
13	J	101	SPO	C17-C19-C20-C21
13	3	102	SPO	C12-C14-C15-C16
13	9	102	SPO	C12-C14-C15-C16
13	9	102	SPO	C17-C19-C20-C21
13	D	103	SPO	C1-C4-C5-C6
13	J	101	SPO	C1-C4-C5-C6
13	O	102	SPO	C1-C4-C5-C6
13	0	101	SPO	C1-C4-C5-C6
8	J	102	BCL	C4-C3-C5-C6
8	8	101	BCL	C2-C1-O2A-CGA
8	9	101	BCL	C2C-C3C-CAC-CBC
8	S	101	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	C	101	BCL	C11-C10-C8-C9
14	M	406	CDL	C55-C56-C57-C58
10	L	306	PC1	C2-C1-O11-P
13	3	102	SPO	C35-C36-C37-C38
8	F	101	BCL	C8-C10-C11-C12
8	O	103	BCL	C10-C11-C12-C13
13	B	101	SPO	C12-C14-C15-C16
13	O	102	SPO	C25-C26-C27-C28
13	U	104	SPO	C11-C10-C9-C7
10	A	102	PC1	C36-C37-C38-C39
14	M	406	CDL	C39-C40-C41-C42
8	L	302	BCL	C4C-C3C-CAC-CBC
13	J	101	SPO	C32-C33-C35-C36
11	M	404	U10	C5-C4-O4-C4M
9	M	403	BPB	C6-C7-C8-C9
13	O	104	SPO	C29-C28-C30-C31
8	U	103	BCL	C11-C12-C13-C15
8	7	101	BCL	C12-C13-C15-C16
13	D	102	SPO	C25-C26-C27-C28
8	O	103	BCL	CAA-CBA-CGA-O2A
8	U	103	BCL	CAA-CBA-CGA-O2A
8	R	101	BCL	C4-C3-C5-C6
13	D	103	SPO	C34-C33-C35-C36
13	O	102	SPO	C29-C28-C30-C31
10	D	104	PC1	O22-C21-O21-C2
10	H	302	PC1	C11-O13-P-O11
13	3	104	SPO	C27-C28-C30-C31
8	3	103	BCL	CAA-CBA-CGA-O2A
10	A	102	PC1	C32-C33-C34-C35
8	L	302	BCL	CAD-CBD-CGD-O2D
8	L	307	BCL	CAD-CBD-CGD-O2D
8	8	101	BCL	CAA-CBA-CGA-O2A
13	U	104	SPO	C34-C33-C35-C36
8	J	102	BCL	C2-C3-C5-C6
11	Y	501	U10	C23-C24-C26-C27
13	O	102	SPO	C27-C28-C30-C31
13	X	101	SPO	C5-C6-C7-C9
10	H	303	PC1	O11-C1-C2-O21
8	F	103	BCL	CAA-CBA-CGA-O2A
8	S	102	BCL	CAA-CBA-CGA-O2A
8	O	103	BCL	O2A-C1-C2-C3
8	L	301	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	M	406	CDL	C44-C45-C46-C47
10	A	102	PC1	O32-C31-O31-C3
13	F	102	SPO	C12-C14-C15-C16
8	C	101	BCL	CAA-CBA-CGA-O2A
13	D	103	SPO	C31-C32-C33-C35
8	R	101	BCL	CAA-CBA-CGA-O2A
10	A	102	PC1	O31-C31-C32-C33
10	A	104	PC1	C11-C12-N-C13
13	3	102	SPO	C2-C1-C4-C5
13	9	102	SPO	C3-C1-C4-C5
13	9	102	SPO	C29-C28-C30-C31
8	7	101	BCL	C14-C13-C15-C16
10	W	101	PC1	C2-C3-O31-C31
13	J	101	SPO	C33-C35-C36-C37
8	C	101	BCL	C13-C15-C16-C17
11	M	404	U10	C3-C4-O4-C4M
13	V	101	SPO	C30-C31-C32-C33
13	X	101	SPO	C30-C31-C32-C33
8	F	103	BCL	CAA-CBA-CGA-O1A
13	9	102	SPO	O1-C1-C4-C5
10	L	304	PC1	C28-C29-C2A-C2B
8	C	101	BCL	CAA-CBA-CGA-O1A
8	S	102	BCL	C1A-C2A-CAA-CBA
8	0	102	BCL	C1A-C2A-CAA-CBA
8	S	102	BCL	CAA-CBA-CGA-O1A
8	J	102	BCL	CAA-CBA-CGA-O2A
11	Y	501	U10	C26-C27-C28-C29
10	A	102	PC1	C32-C31-O31-C3
8	O	103	BCL	CAA-CBA-CGA-O1A
8	U	103	BCL	CAA-CBA-CGA-O1A
8	3	103	BCL	CAA-CBA-CGA-O1A
8	8	101	BCL	CAA-CBA-CGA-O1A
10	L	306	PC1	C1-O11-P-O12
10	A	102	PC1	C11-O13-P-O12
10	A	104	PC1	C1-O11-P-O12
11	Y	501	U10	C6-C7-C8-C9
8	7	101	BCL	CAA-CBA-CGA-O2A
8	R	101	BCL	CAA-CBA-CGA-O1A
8	A	103	BCL	CAA-CBA-CGA-O2A
8	U	101	BCL	C8-C10-C11-C12
14	H	304	CDL	C53-C54-C55-C56
13	D	103	SPO	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
8	W	102	BCL	C6-C7-C8-C9
10	A	102	PC1	O32-C31-C32-C33
8	N	101	BCL	CAA-CBA-CGA-O2A
13	O	104	SPO	C1-C4-C5-C6
8	J	102	BCL	CAA-CBA-CGA-O1A
8	E	101	BCL	CAA-CBA-CGA-O2A
8	U	103	BCL	C8-C10-C11-C12
8	L	307	BCL	C6-C7-C8-C10
13	I	102	SPO	C32-C33-C35-C36
13	O	104	SPO	C27-C28-C30-C31
8	E	101	BCL	CAA-CBA-CGA-O1A
13	8	102	SPO	C11-C10-C9-C7
10	H	302	PC1	C32-C33-C34-C35
11	M	404	U10	C24-C26-C27-C28
13	U	102	SPO	C28-C30-C31-C32
10	D	104	PC1	C22-C21-O21-C2
14	H	304	CDL	C51-C52-C53-C54
8	7	101	BCL	CAA-CBA-CGA-O1A
11	Y	501	U10	C12-C11-C9-C10
8	1	102	BCL	CAA-CBA-CGA-O2A
8	0	102	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

72 monomers are involved in 291 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	3	103	BCL	1	0
13	U	102	SPO	8	0
13	X	101	SPO	6	0
8	R	101	BCL	7	0
10	H	302	PC1	5	0
13	O	102	SPO	6	0
11	Y	501	U10	2	0
13	M	405	SPO	7	0
8	L	307	BCL	1	0
13	I	102	SPO	7	0
8	L	302	BCL	4	0
14	M	406	CDL	4	0
8	M	402	BCL	2	0
13	3	104	SPO	7	0
10	D	104	PC1	5	0
8	L	301	BCL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	102	SPO	4	0
10	L	306	PC1	2	0
8	S	101	BCL	2	0
8	E	101	BCL	2	0
11	M	404	U10	3	0
8	A	101	BCL	1	0
13	T	101	SPO	6	0
8	S	102	BCL	6	0
8	W	102	BCL	4	0
10	L	304	PC1	1	0
8	J	102	BCL	6	0
8	I	101	BCL	1	0
8	F	103	BCL	3	0
11	L	308	U10	1	0
8	O	103	BCL	4	0
13	W	103	SPO	7	0
11	L	305	U10	5	0
8	7	101	BCL	10	0
13	0	101	SPO	8	0
13	9	102	SPO	5	0
8	U	101	BCL	6	0
8	Q	101	BCL	2	0
8	U	103	BCL	4	0
10	A	104	PC1	6	0
10	W	101	PC1	5	0
9	L	303	BPB	4	0
13	G	101	SPO	6	0
8	9	101	BCL	3	0
13	3	102	SPO	9	0
8	3	101	BCL	1	0
8	1	101	BCL	1	0
13	P	101	SPO	5	0
13	V	101	SPO	8	0
13	J	101	SPO	3	0
13	J	103	SPO	8	0
10	A	102	PC1	7	0
13	E	102	SPO	4	0
8	N	101	BCL	5	0
8	8	101	BCL	4	0
10	H	301	PC1	6	0
13	D	103	SPO	9	0
13	N	102	SPO	8	0

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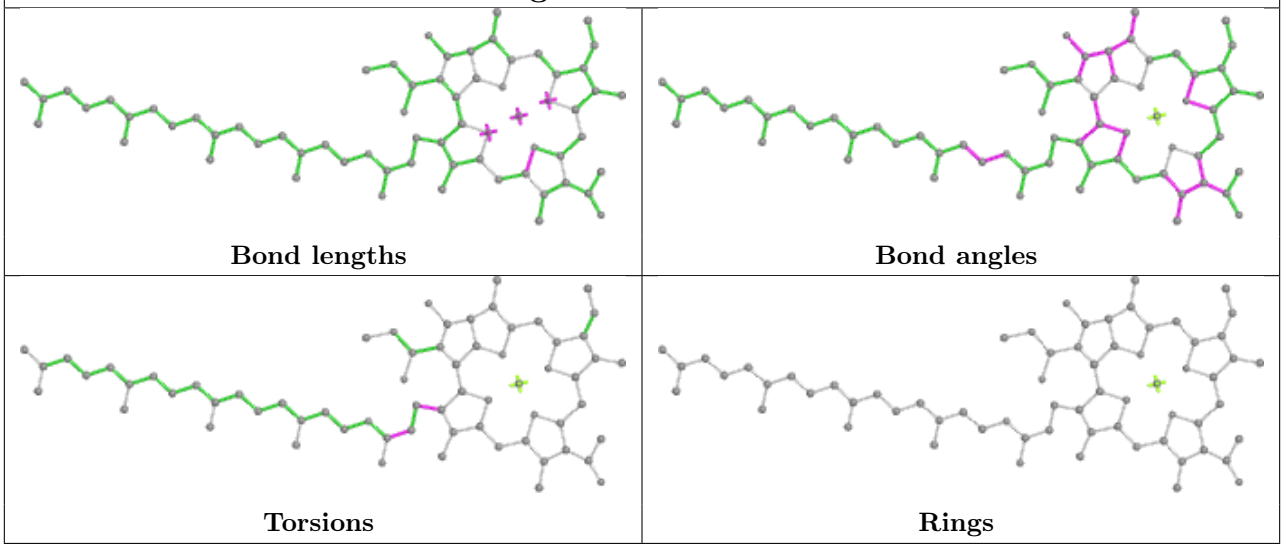
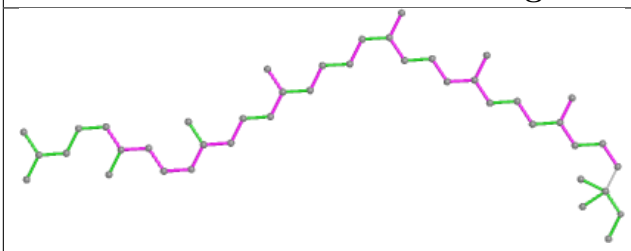
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	102	SPO	10	0
13	8	102	SPO	5	0
8	F	101	BCL	3	0
14	H	304	CDL	6	0
13	O	104	SPO	5	0
13	F	102	SPO	8	0
8	1	102	BCL	2	0
8	0	102	BCL	4	0
9	M	403	BPB	5	0
8	D	101	BCL	2	0
13	B	101	SPO	10	0
8	A	103	BCL	9	0
13	U	104	SPO	4	0
8	C	101	BCL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

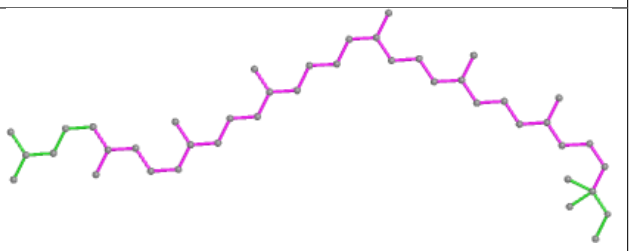
Ligand BCL 3 103



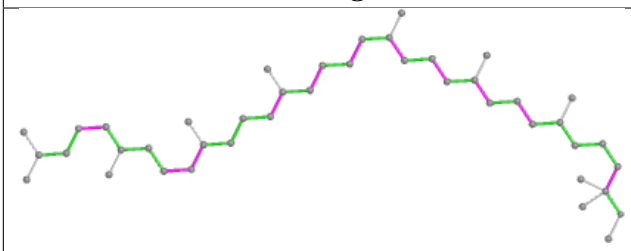
Ligand SPO U 102



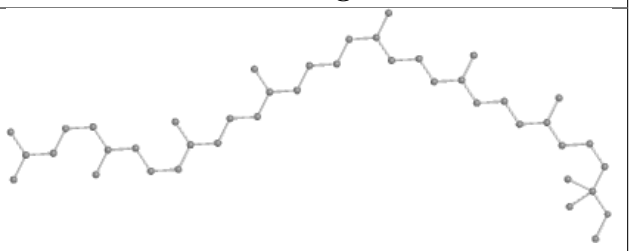
Bond lengths



Bond angles

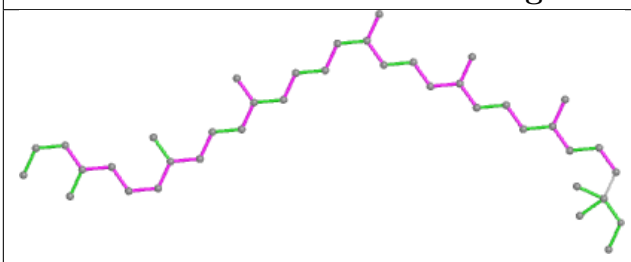


Torsions

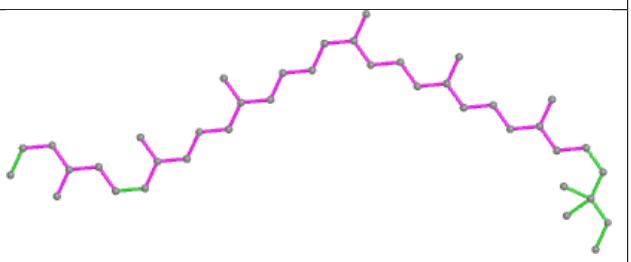


Rings

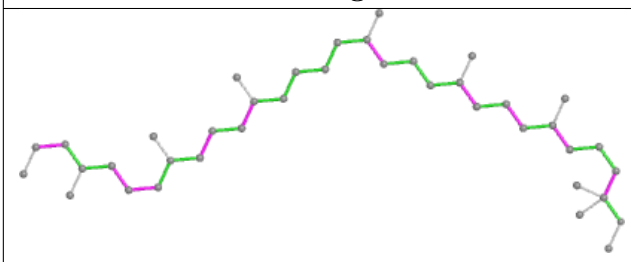
Ligand SPO X 101



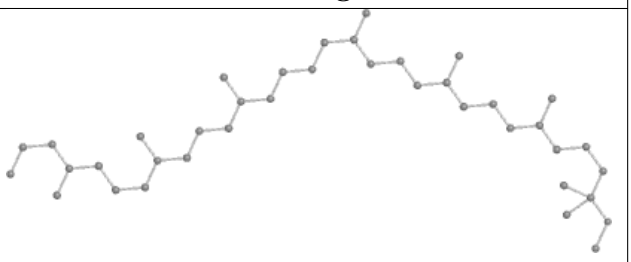
Bond lengths



Bond angles

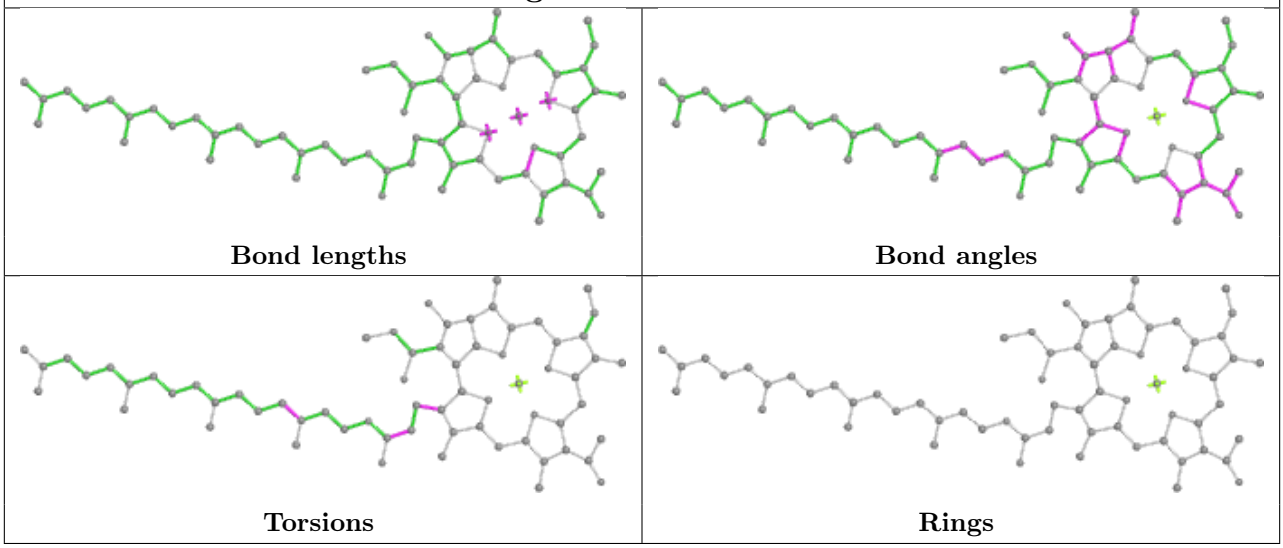


Torsions

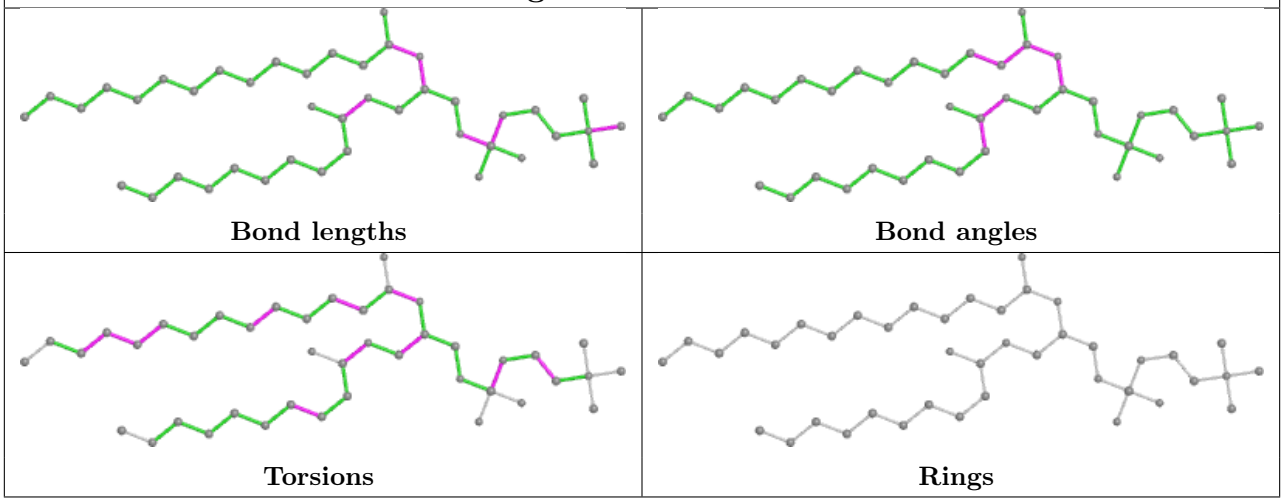


Rings

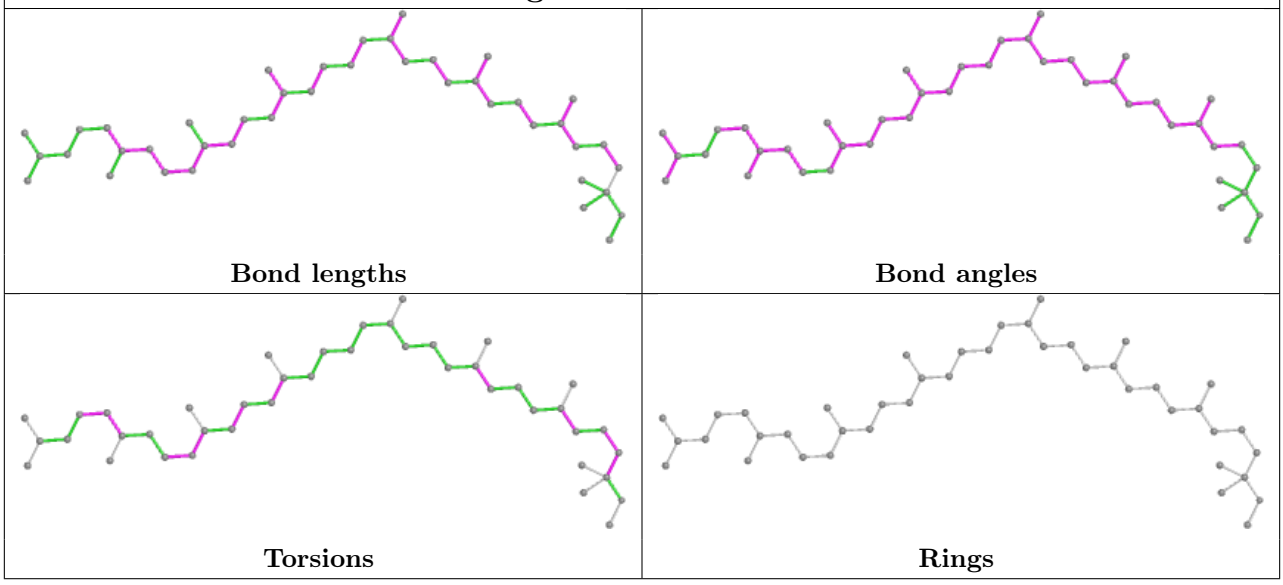
Ligand BCL R 101



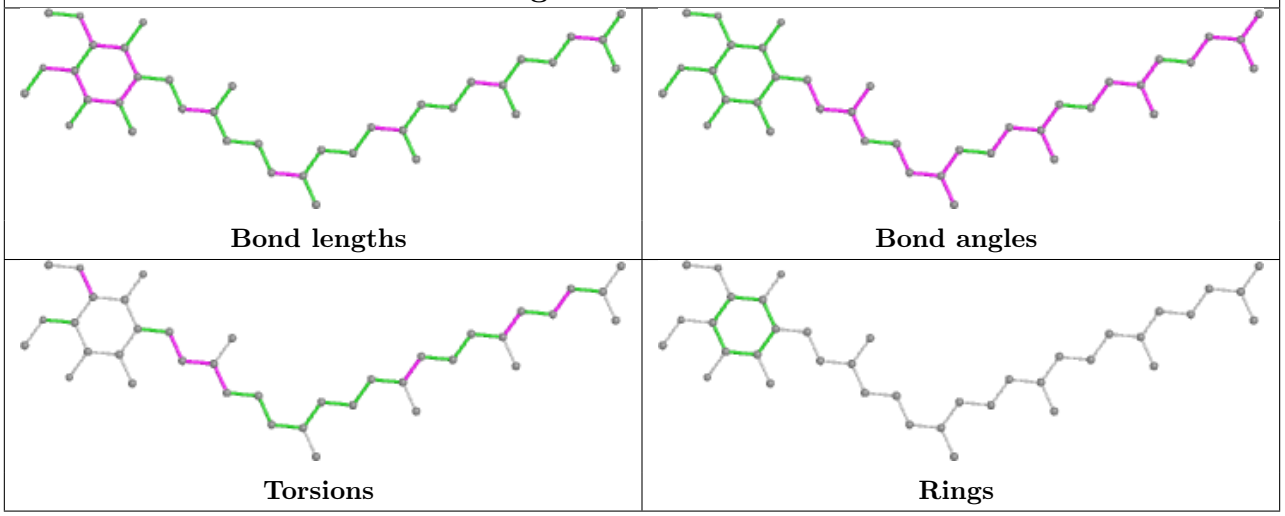
Ligand PC1 H 302



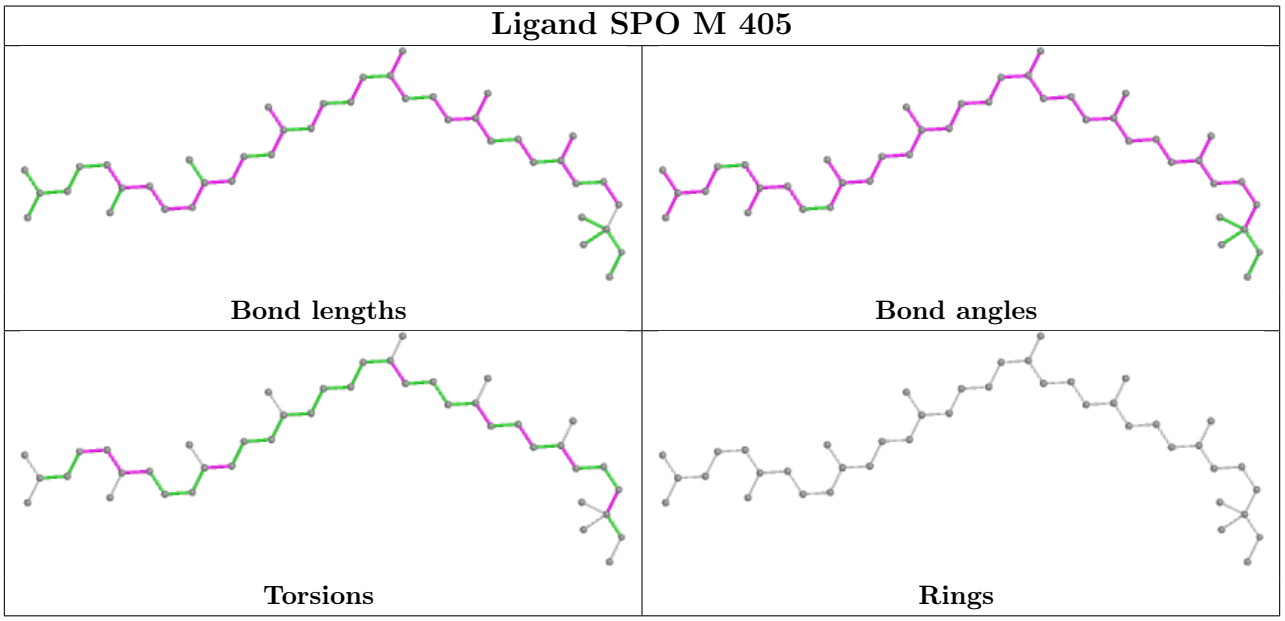
Ligand SPO O 102



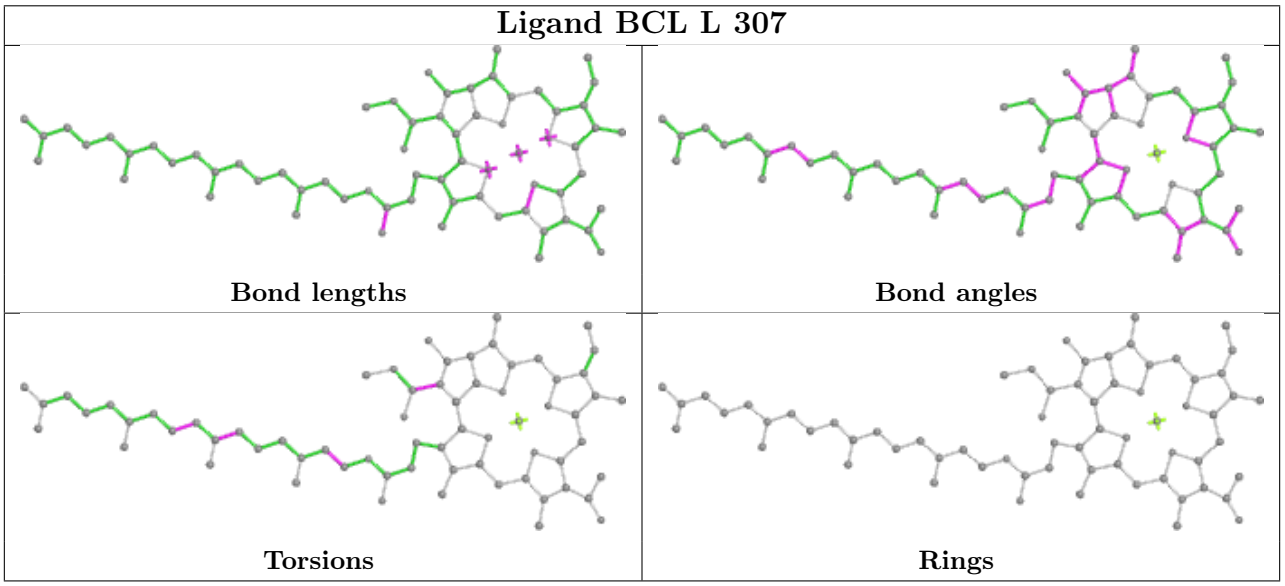
Ligand U10 Y 501



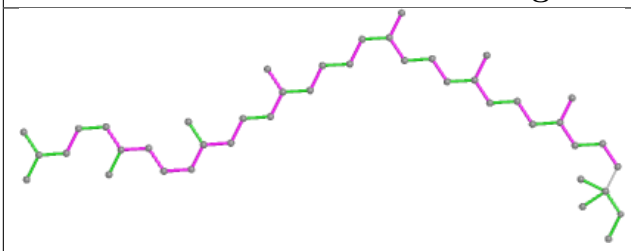
Ligand SPO M 405



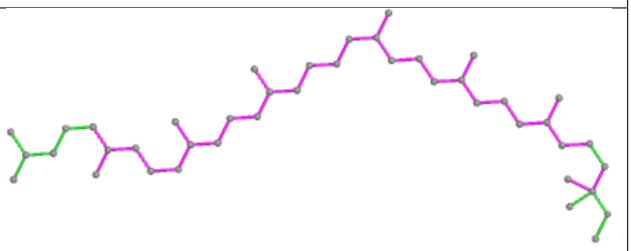
Ligand BCL L 307



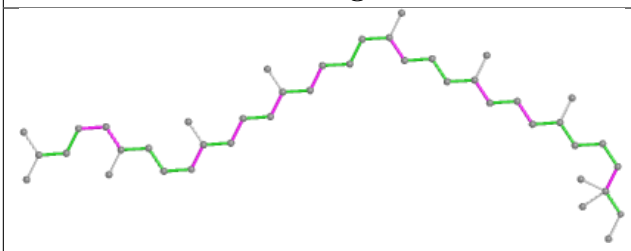
Ligand SPO I 102



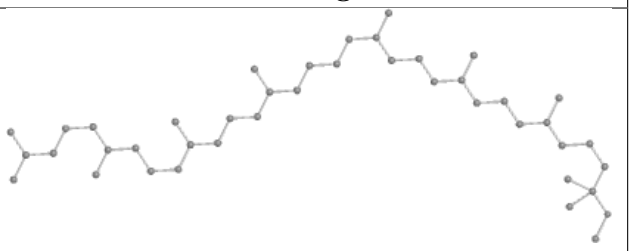
Bond lengths



Bond angles

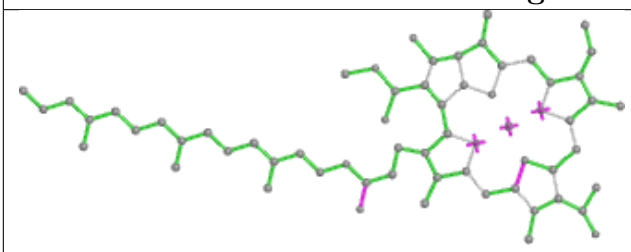


Torsions

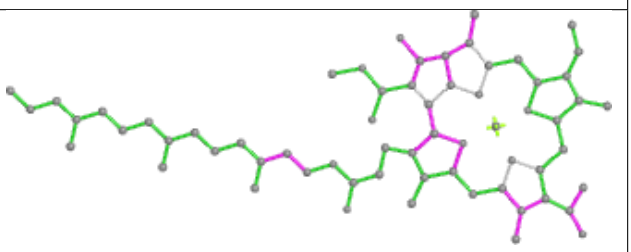


Rings

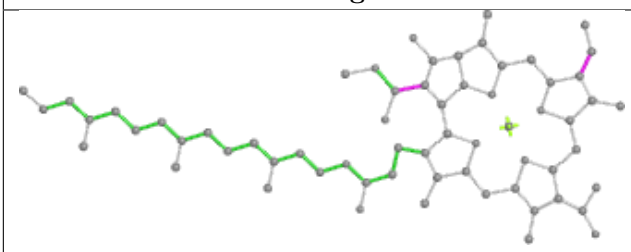
Ligand BCL L 302



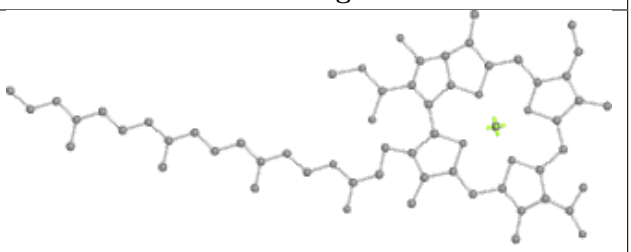
Bond lengths



Bond angles

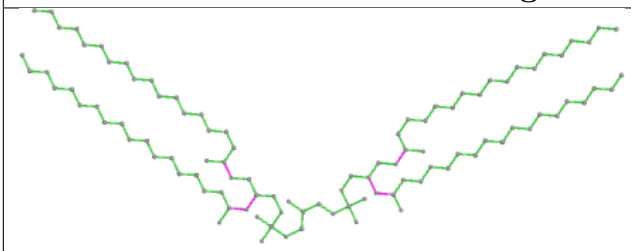


Torsions

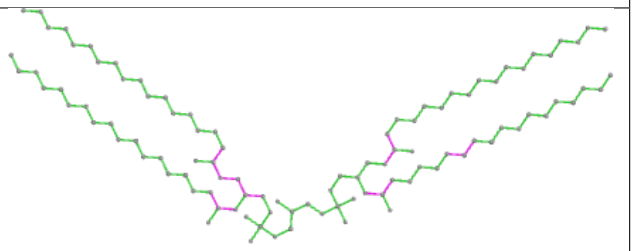


Rings

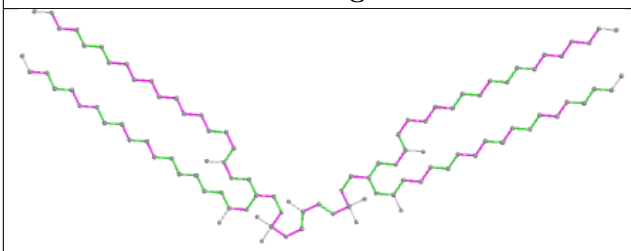
Ligand CDL M 406



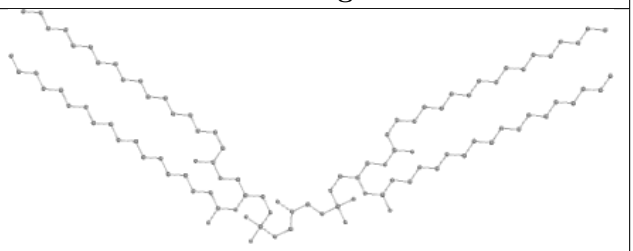
Bond lengths



Bond angles

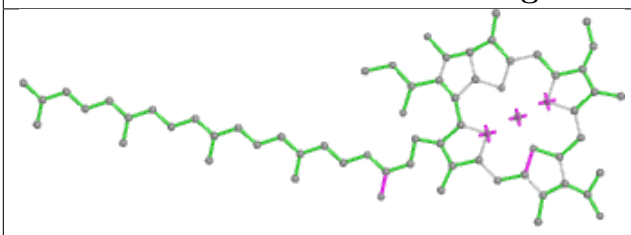


Torsions

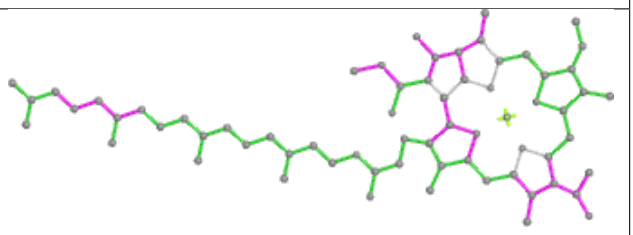


Rings

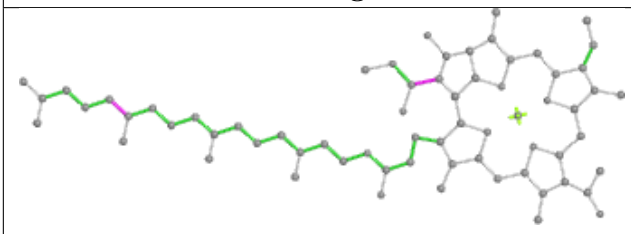
Ligand BCL M 402



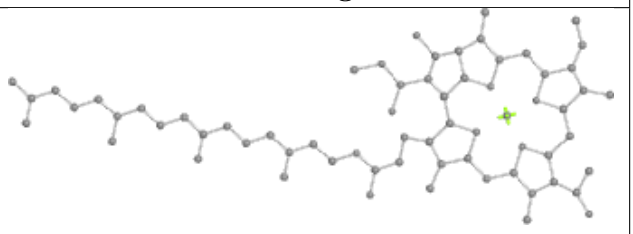
Bond lengths



Bond angles

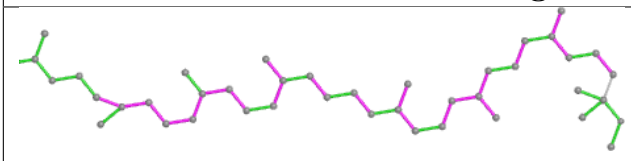


Torsions

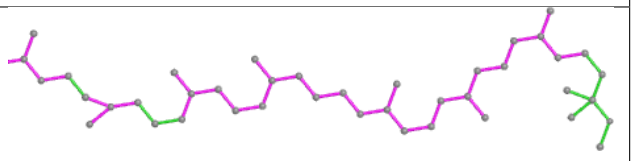


Rings

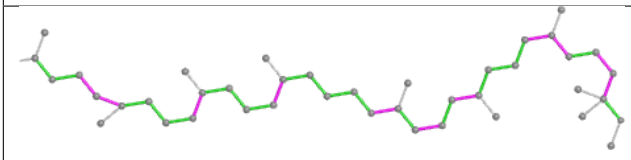
Ligand SPO 3 104



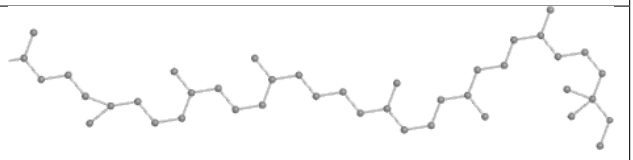
Bond lengths



Bond angles

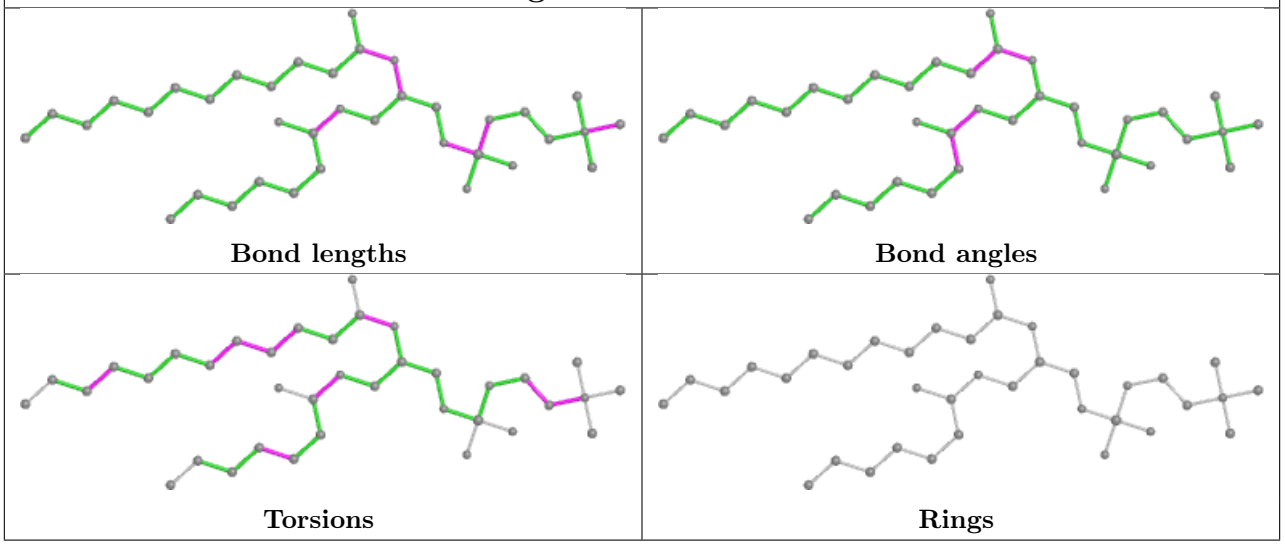


Torsions

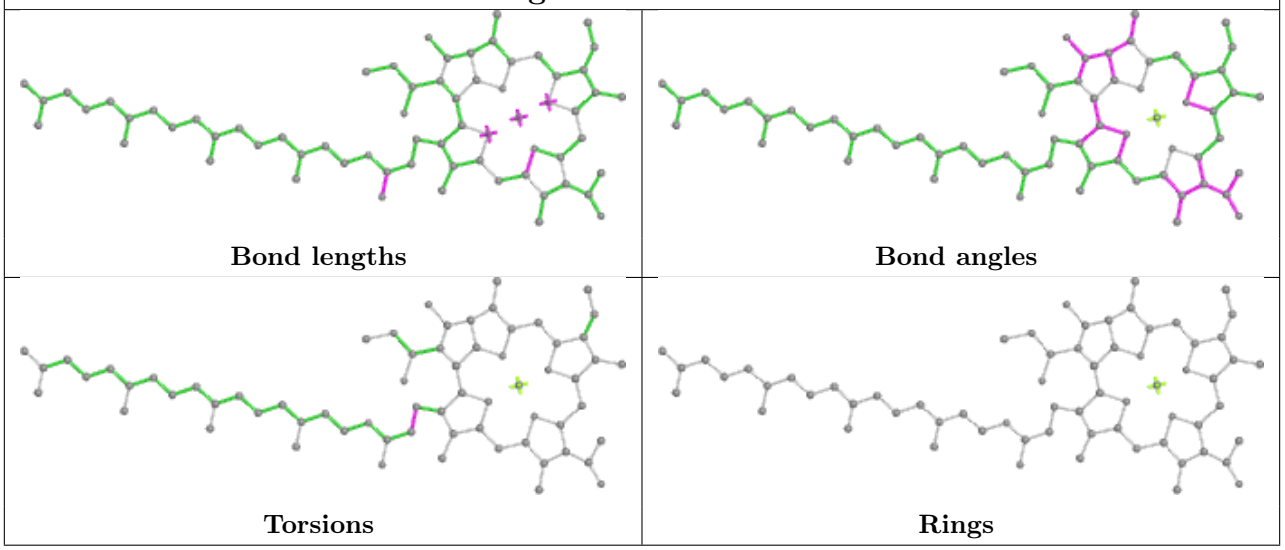


Rings

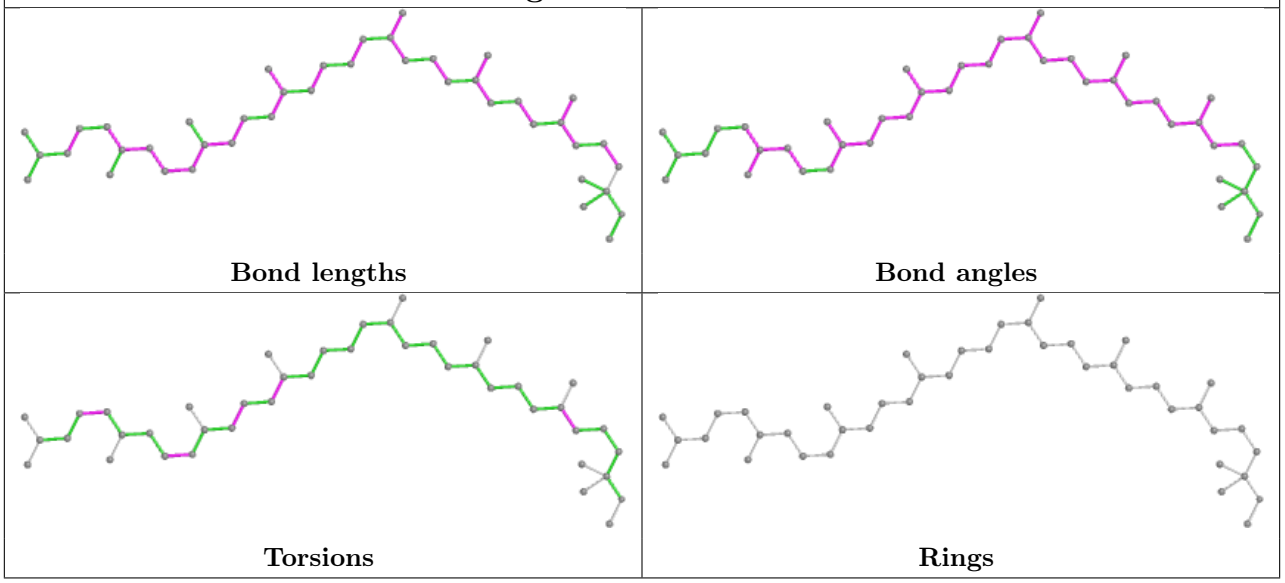
Ligand PC1 D 104



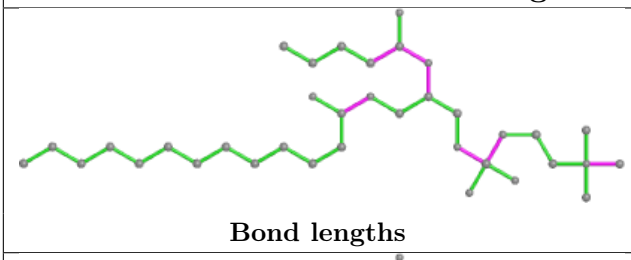
Ligand BCL L 301

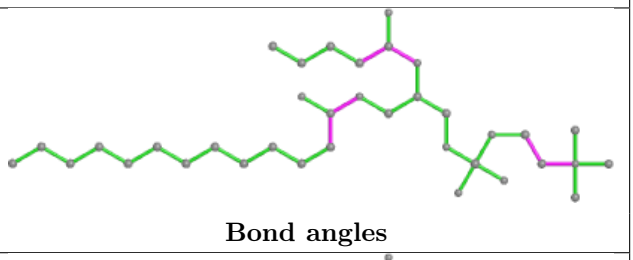


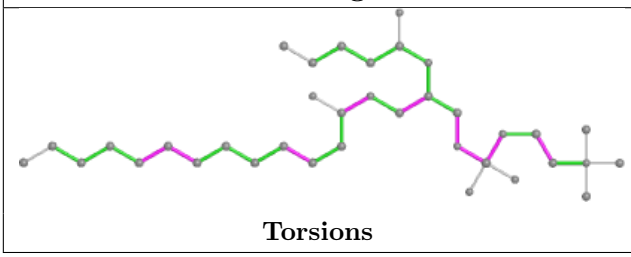
Ligand SPO D 102

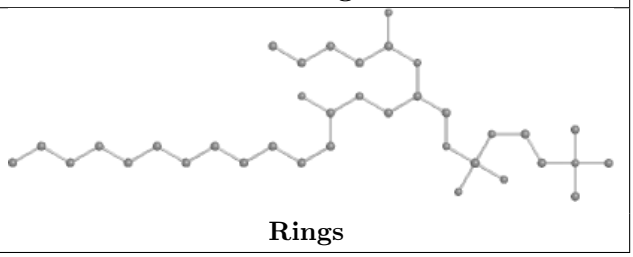


Ligand PC1 L 306

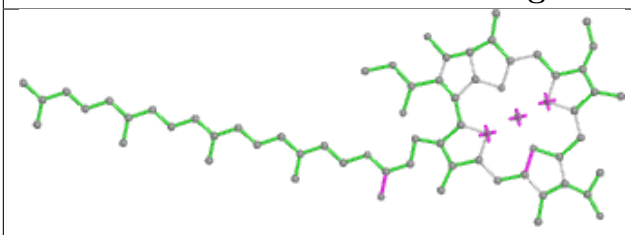

Bond lengths

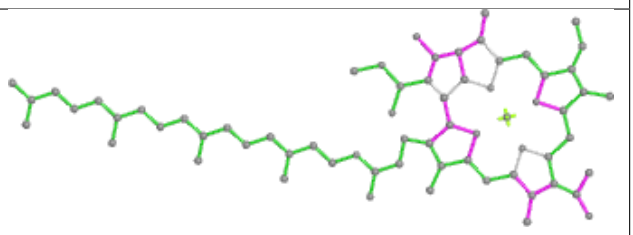

Bond angles

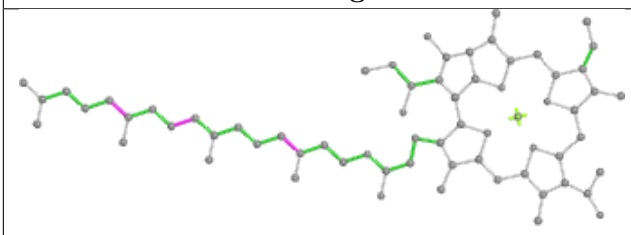

Torsions

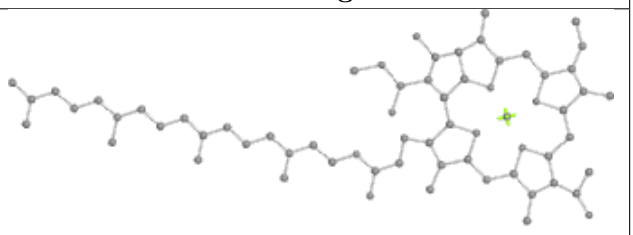

Rings

Ligand BCL S 101

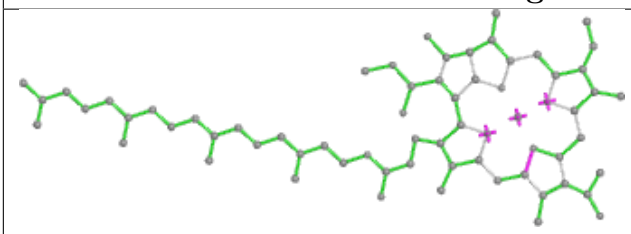

Bond lengths

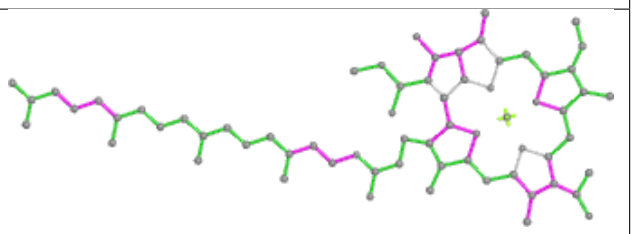

Bond angles

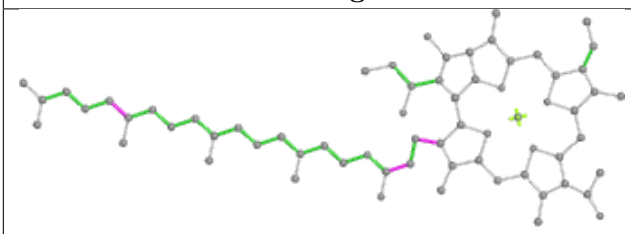

Torsions

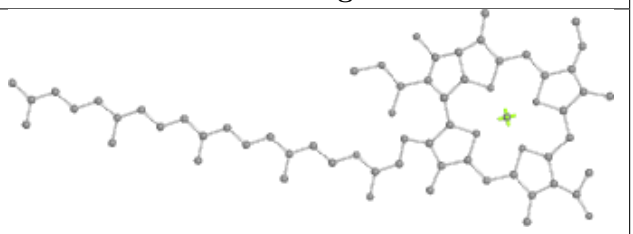

Rings

Ligand BCL E 101

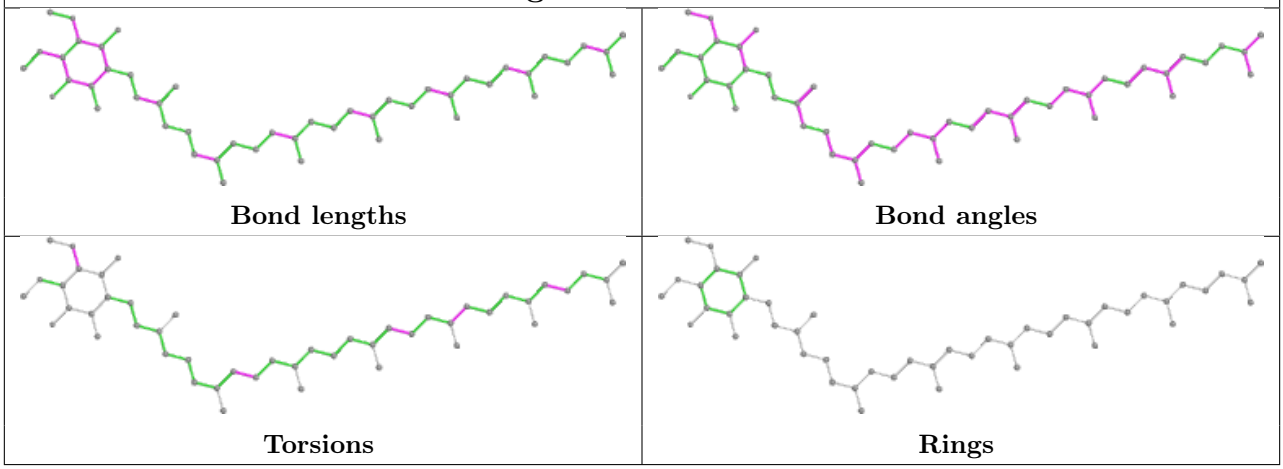

Bond lengths


Bond angles

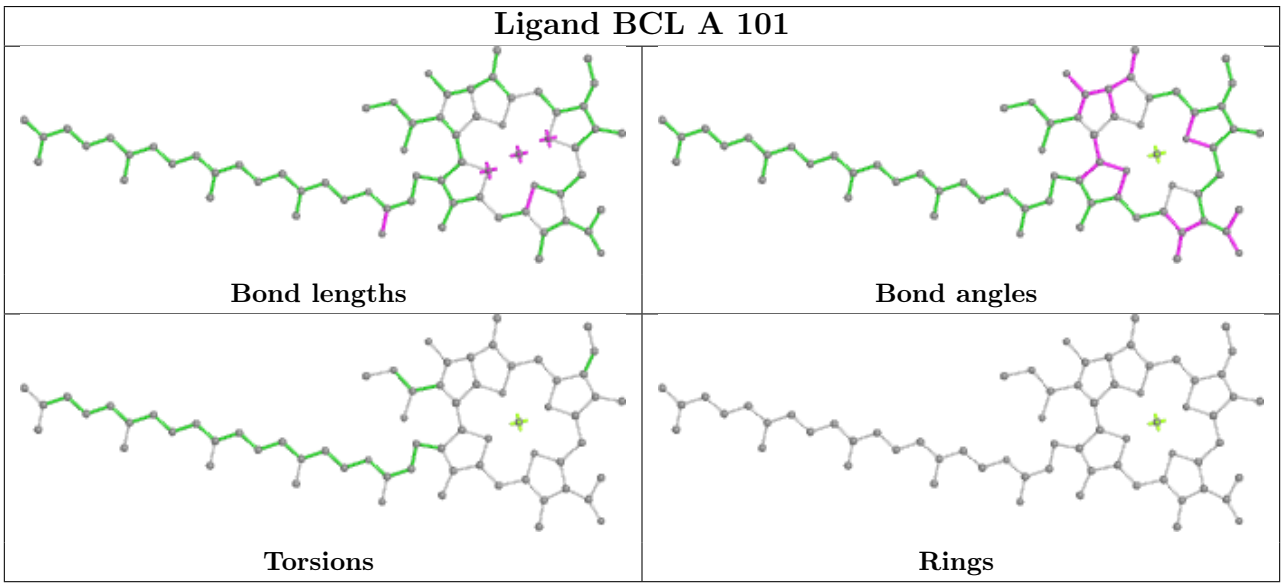

Torsions


Rings

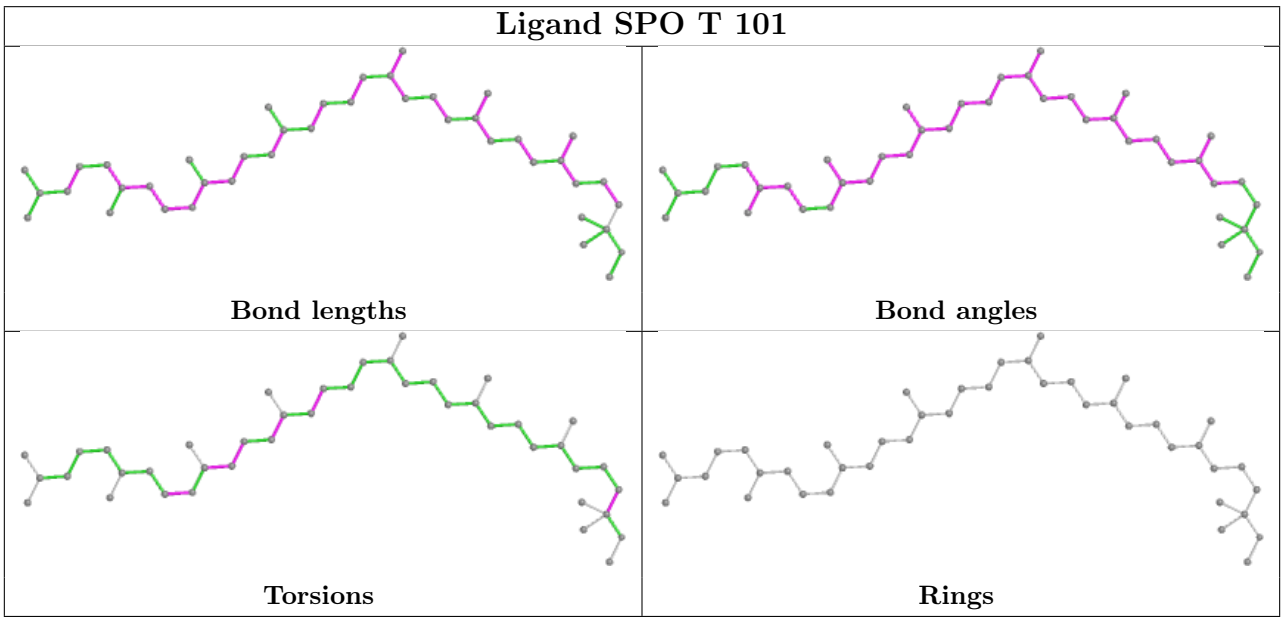
Ligand U10 M 404



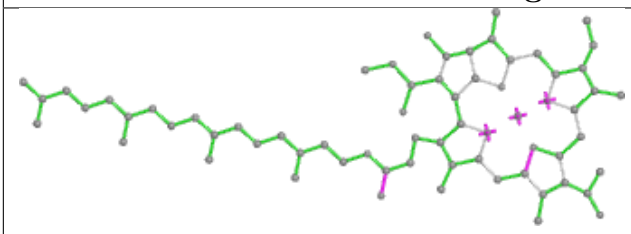
Ligand BCL A 101



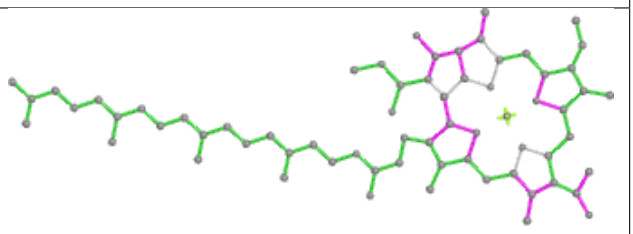
Ligand SPO T 101



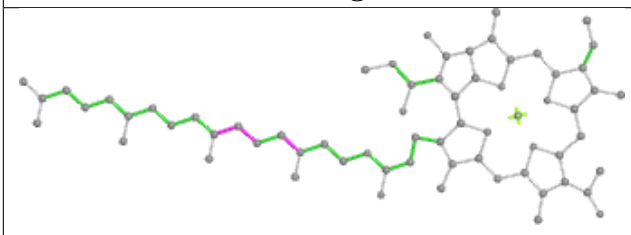
Ligand BCL O 101



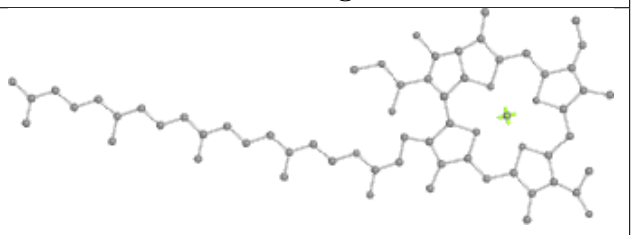
Bond lengths



Bond angles

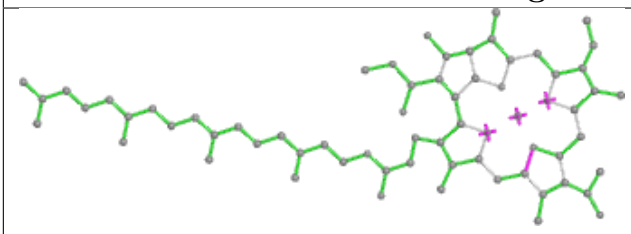


Torsions

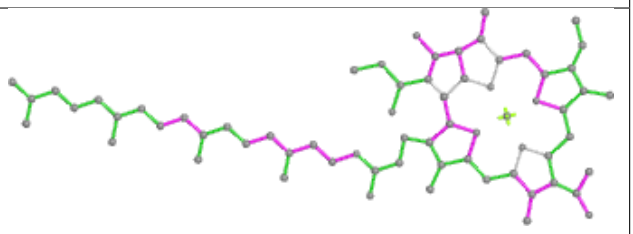


Rings

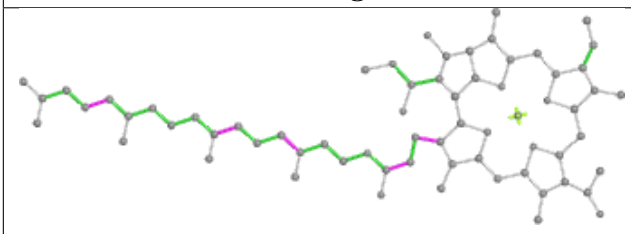
Ligand BCL S 102



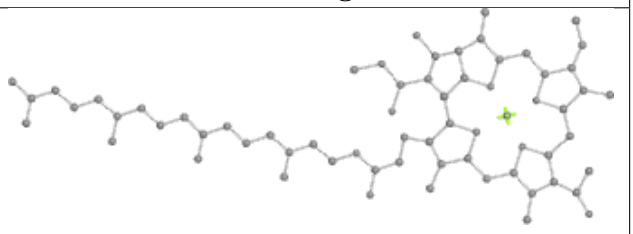
Bond lengths



Bond angles

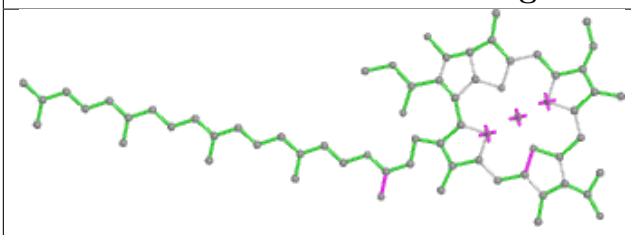


Torsions

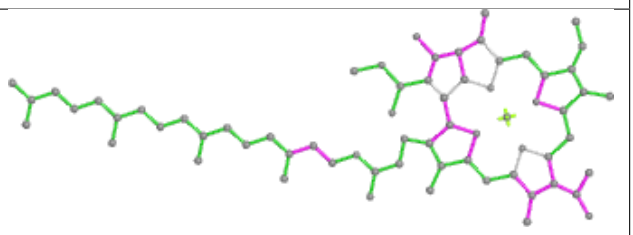


Rings

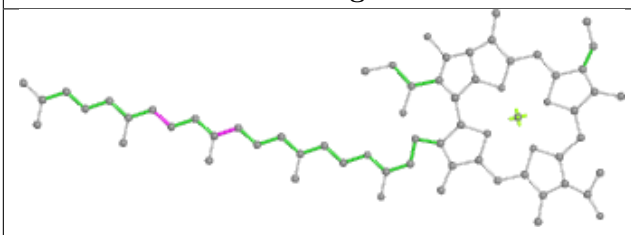
Ligand BCL W 102



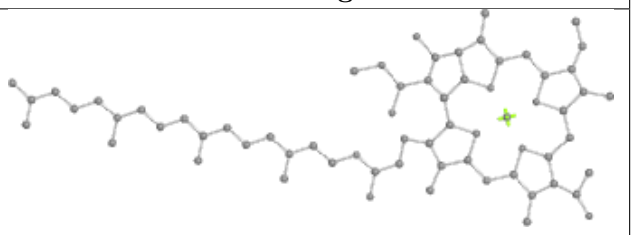
Bond lengths



Bond angles

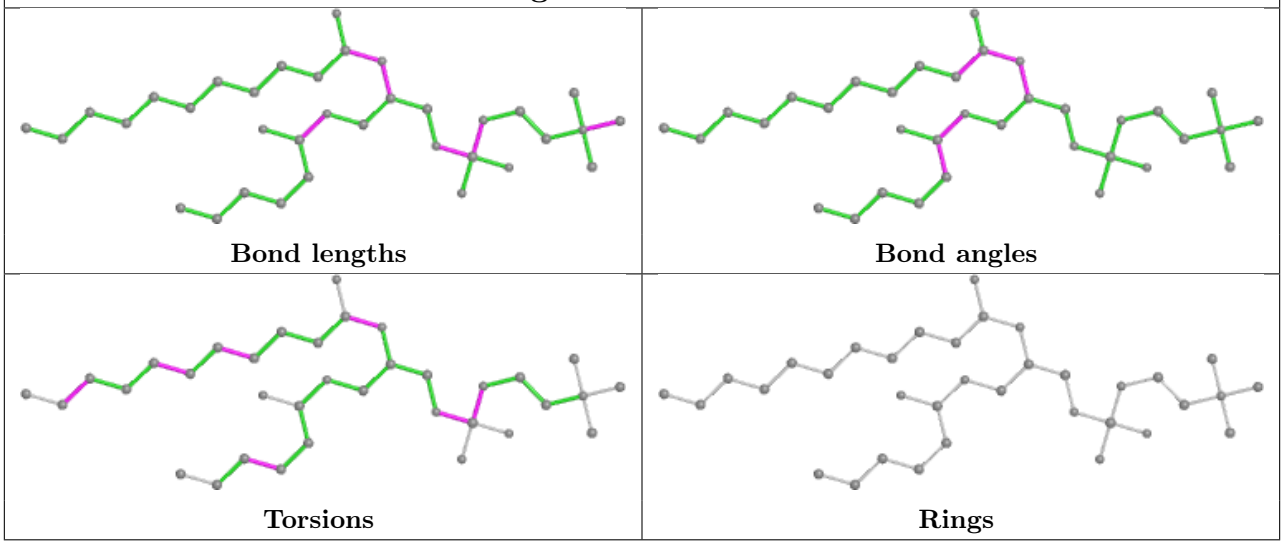


Torsions

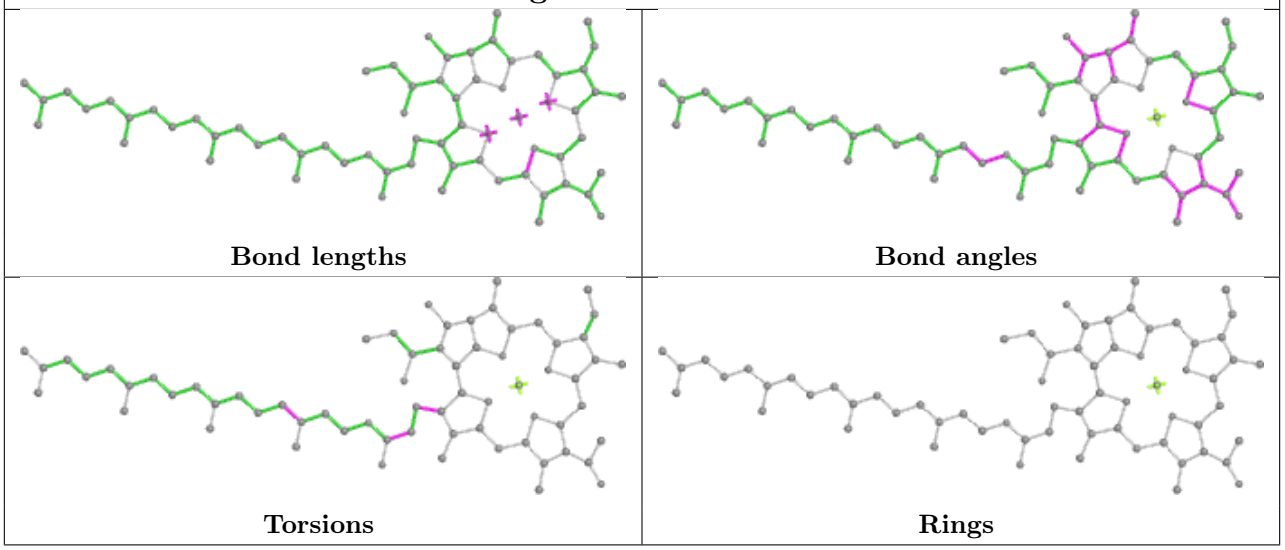


Rings

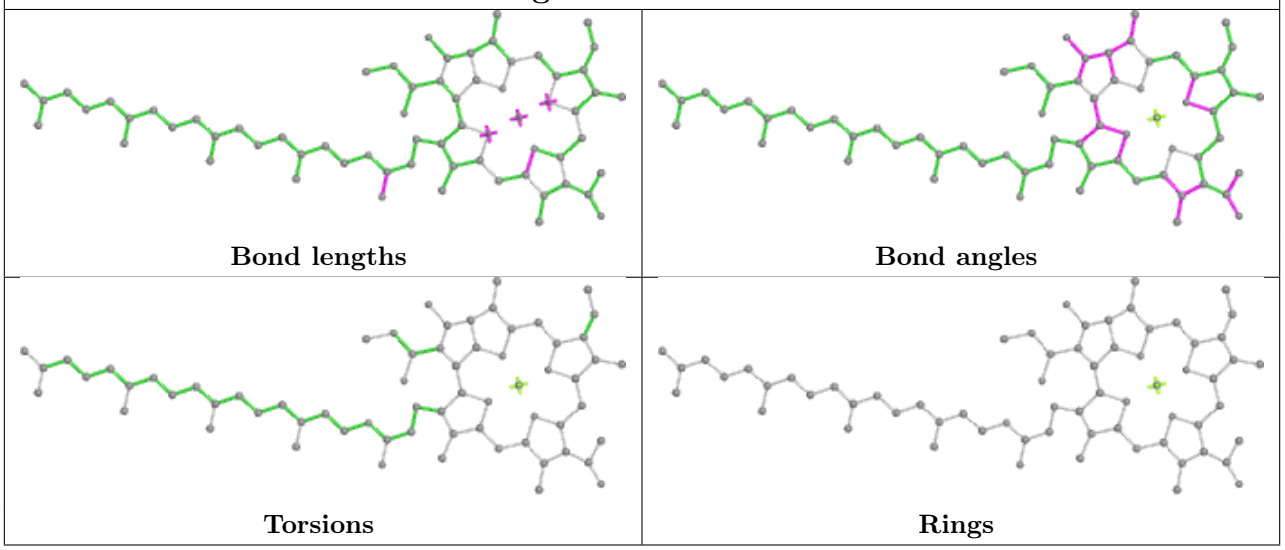
Ligand PC1 L 304



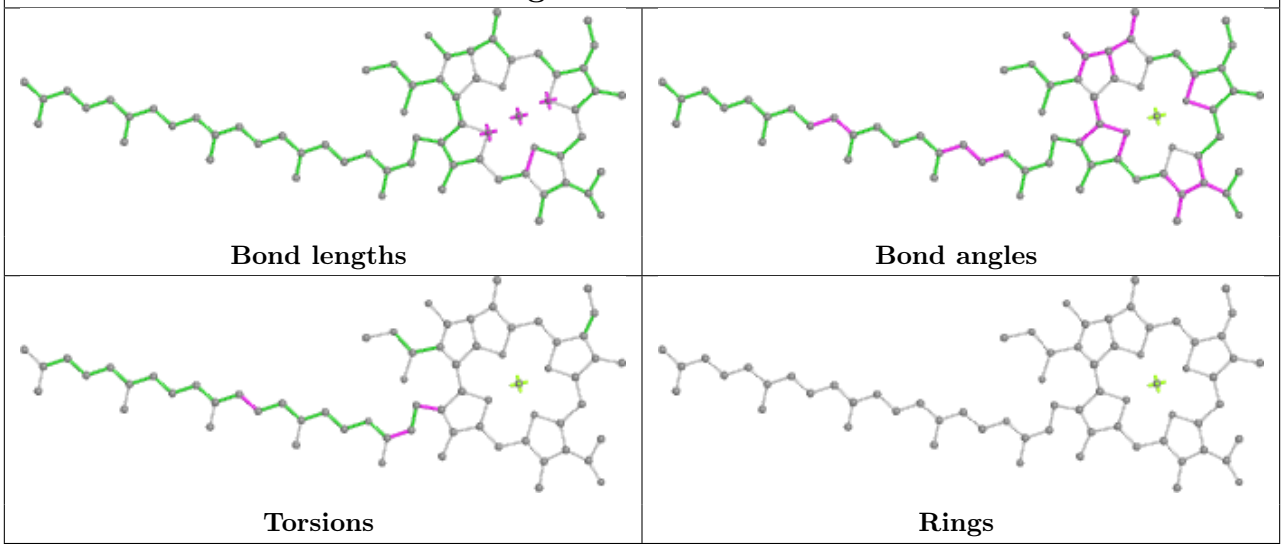
Ligand BCL J 102



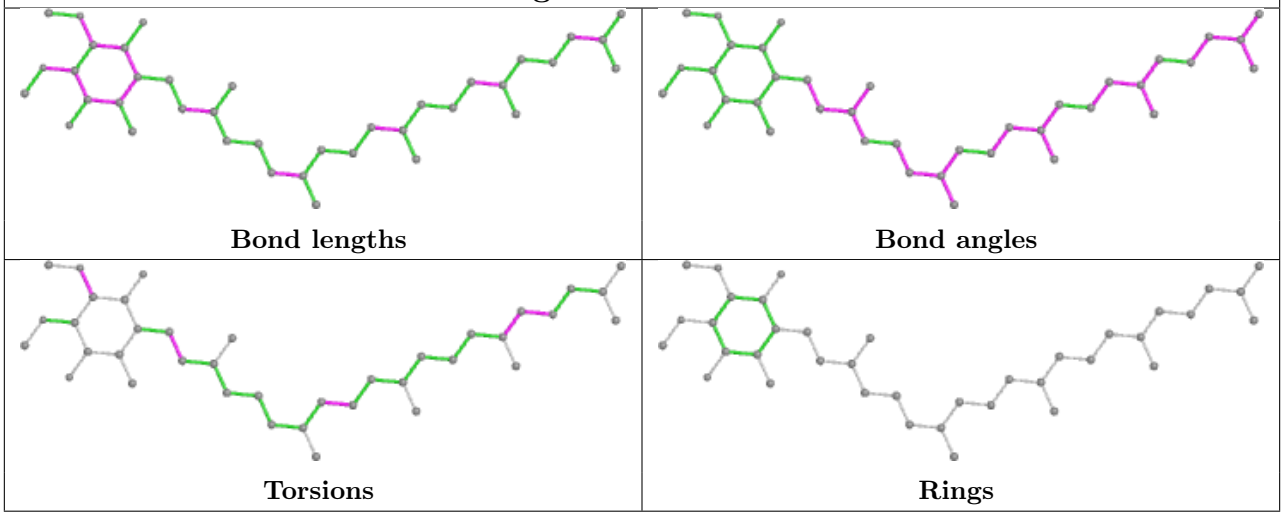
Ligand BCL I 101



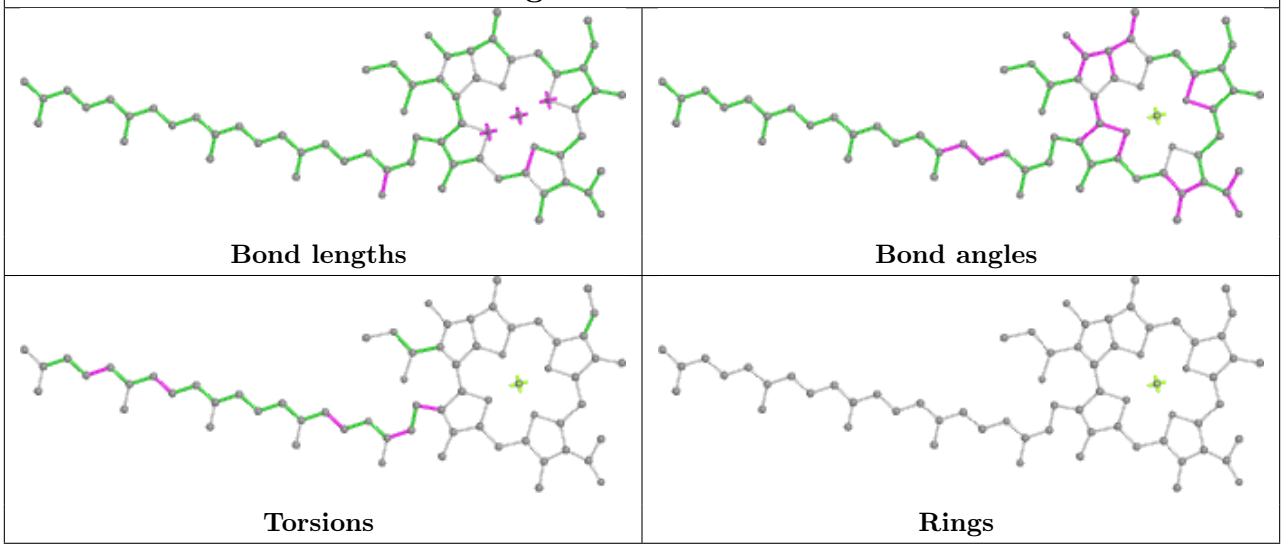
Ligand BCL F 103



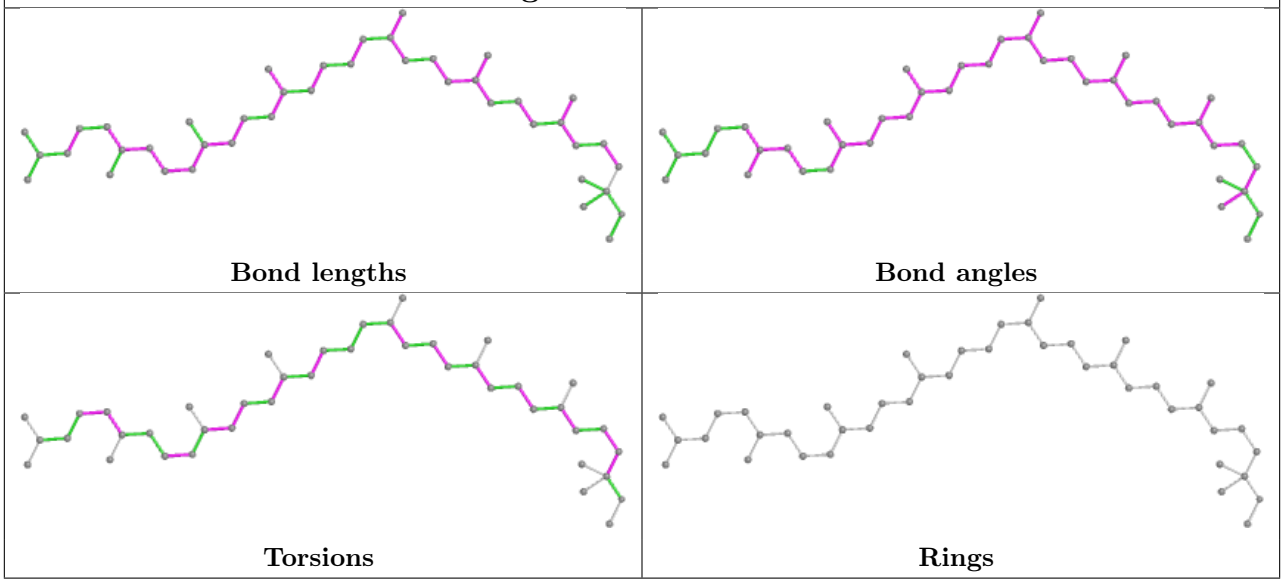
Ligand U10 L 308



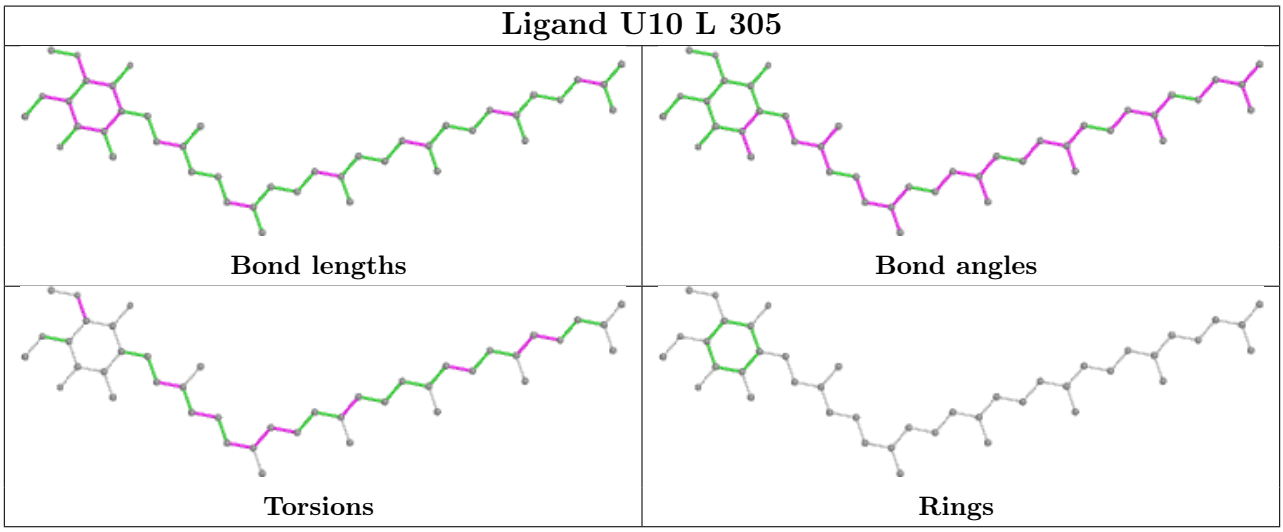
Ligand BCL O 103



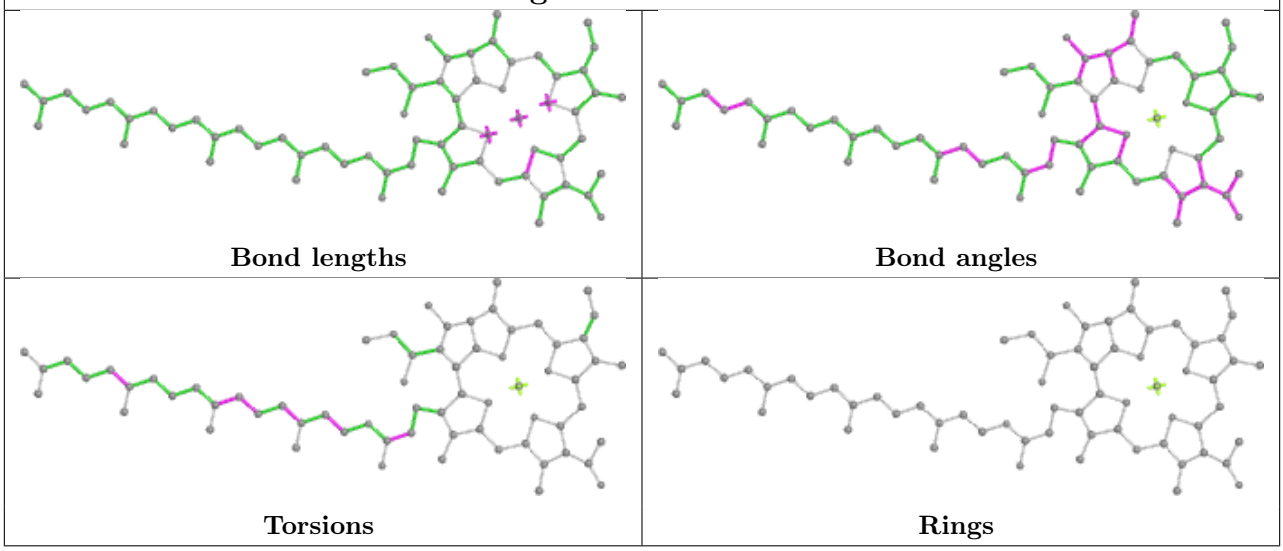
Ligand SPO W 103



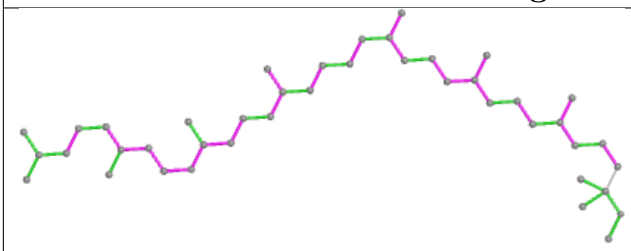
Ligand U10 L 305



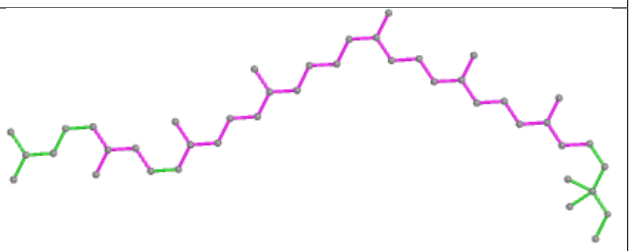
Ligand BCL 7 101



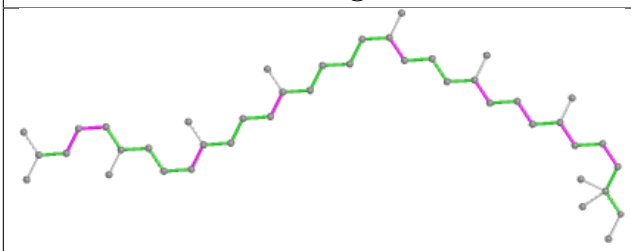
Ligand SPO 0 101



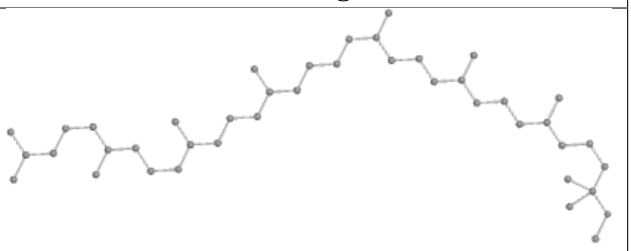
Bond lengths



Bond angles

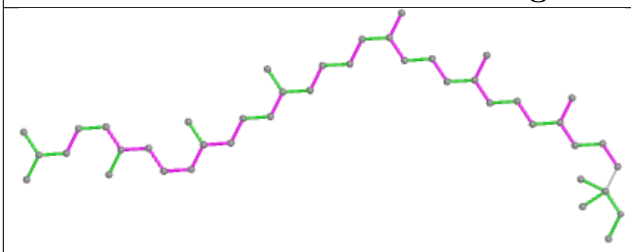


Torsions



Rings

Ligand SPO 9 102



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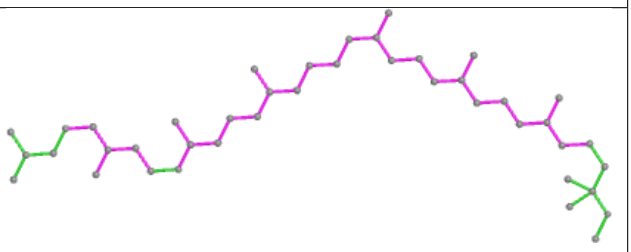
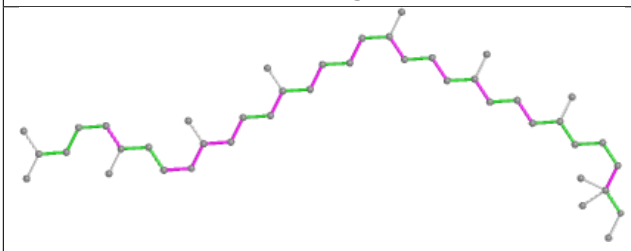
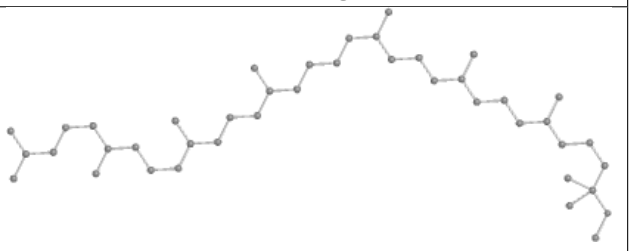


Bond angles

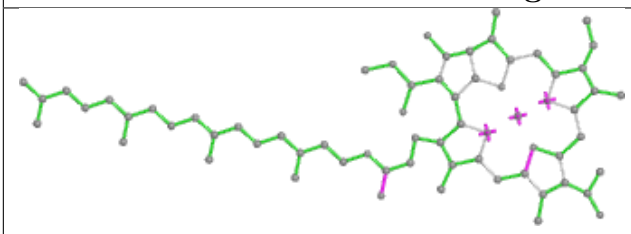


Torsions

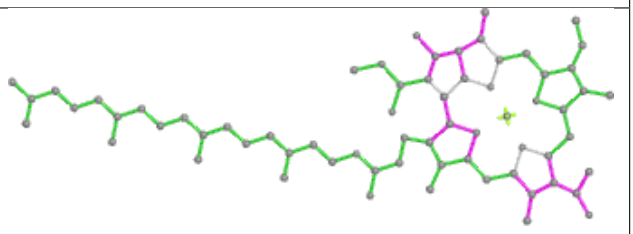


Rings

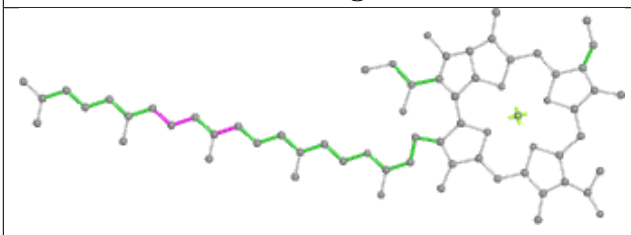
Ligand BCL U 101



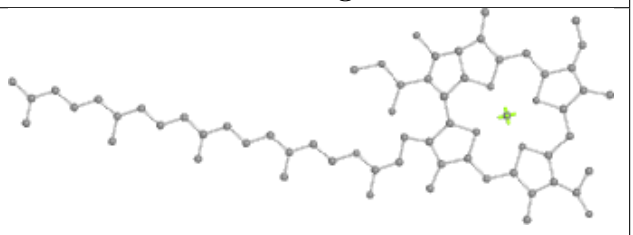
Bond lengths



Bond angles

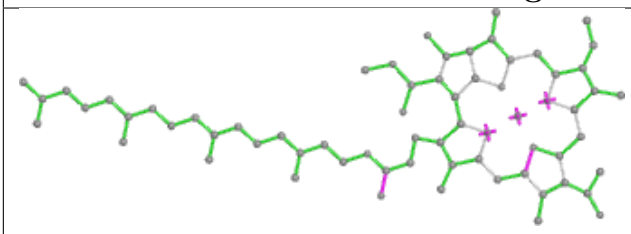


Torsions

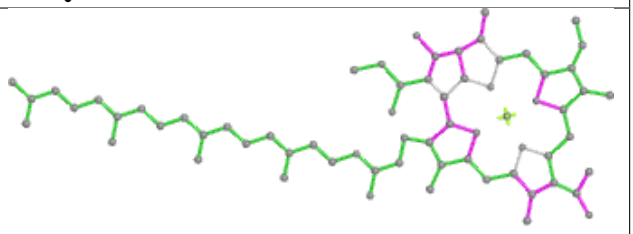


Rings

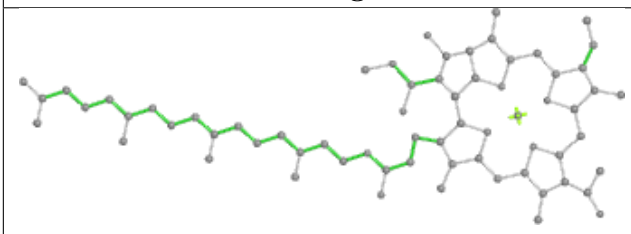
Ligand BCL Q 101



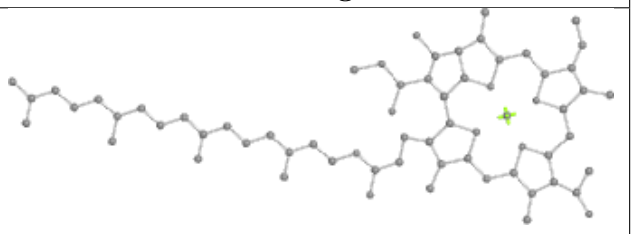
Bond lengths



Bond angles

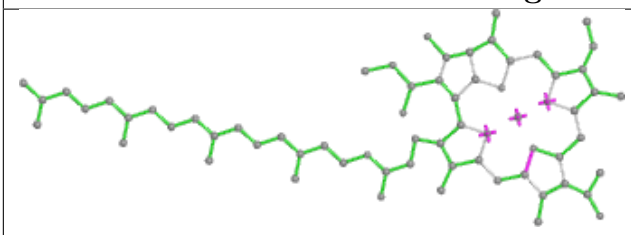


Torsions

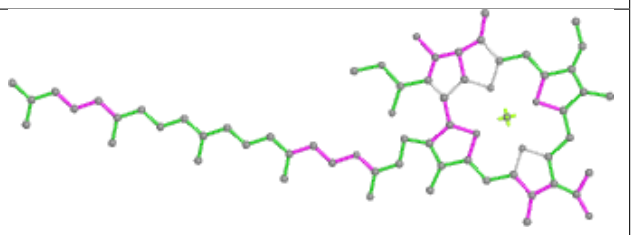


Rings

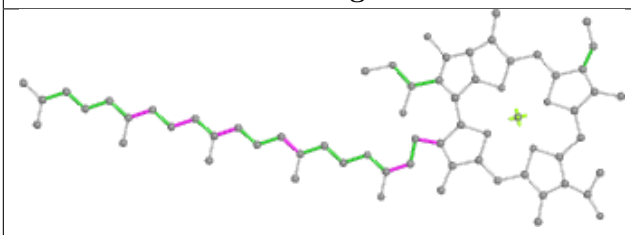
Ligand BCL U 103



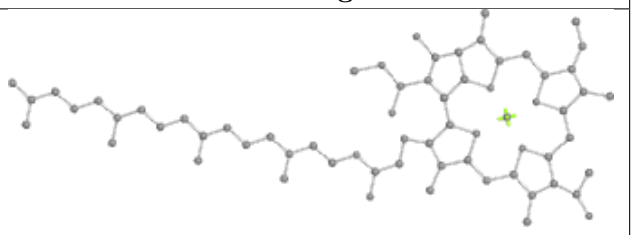
Bond lengths



Bond angles

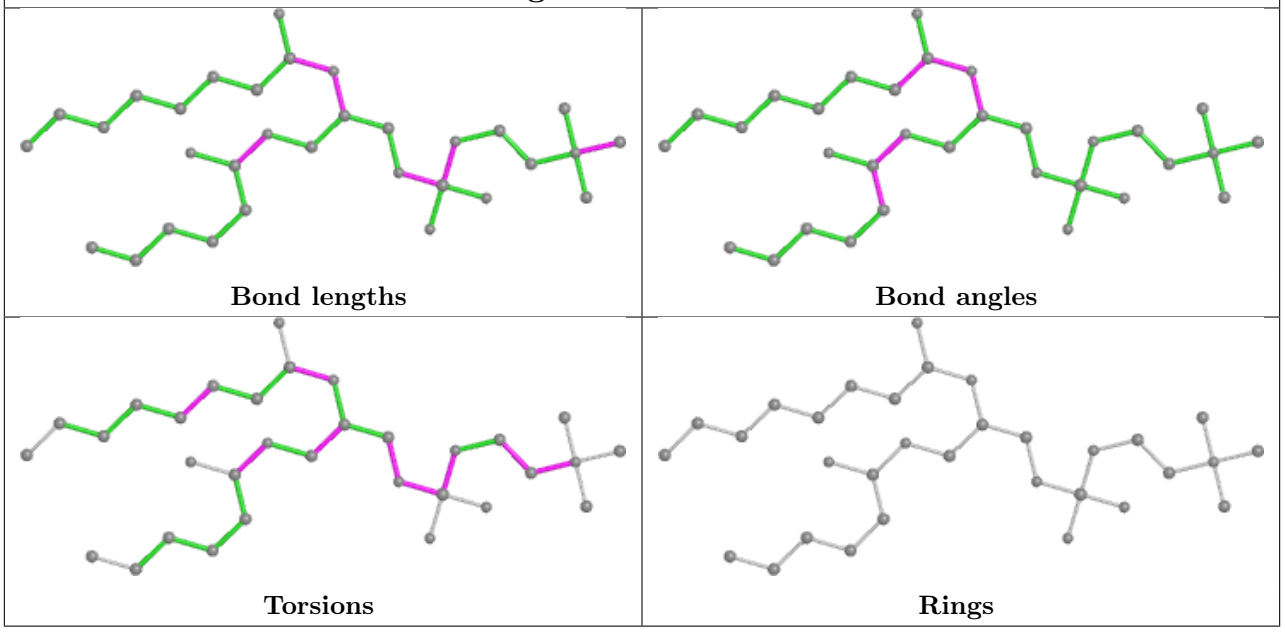


Torsions

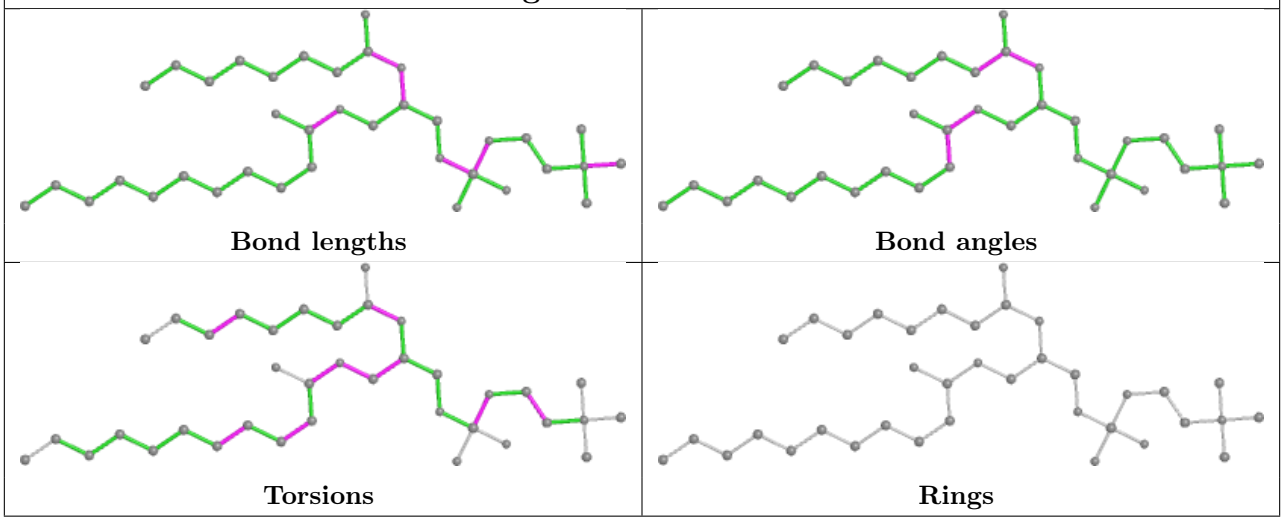


Rings

Ligand PC1 A 104

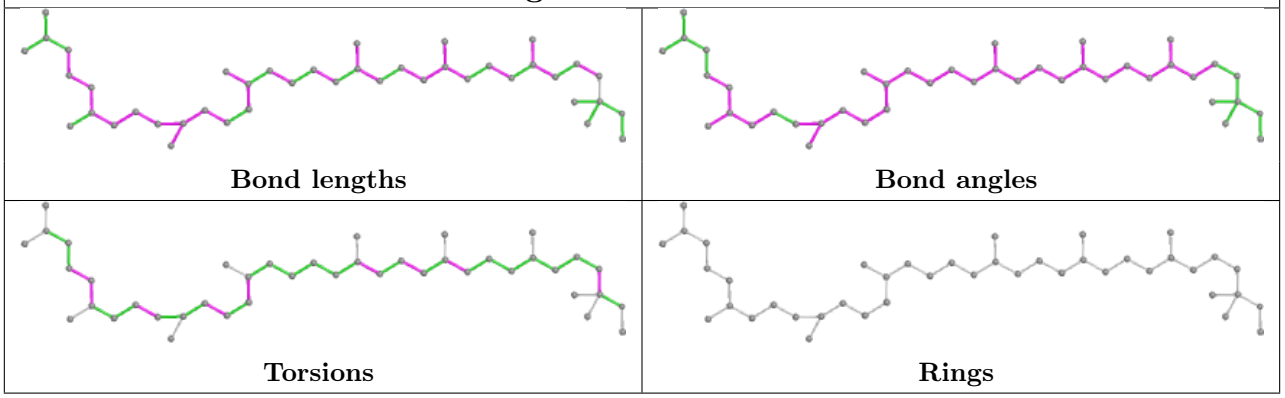


Ligand PC1 W 101

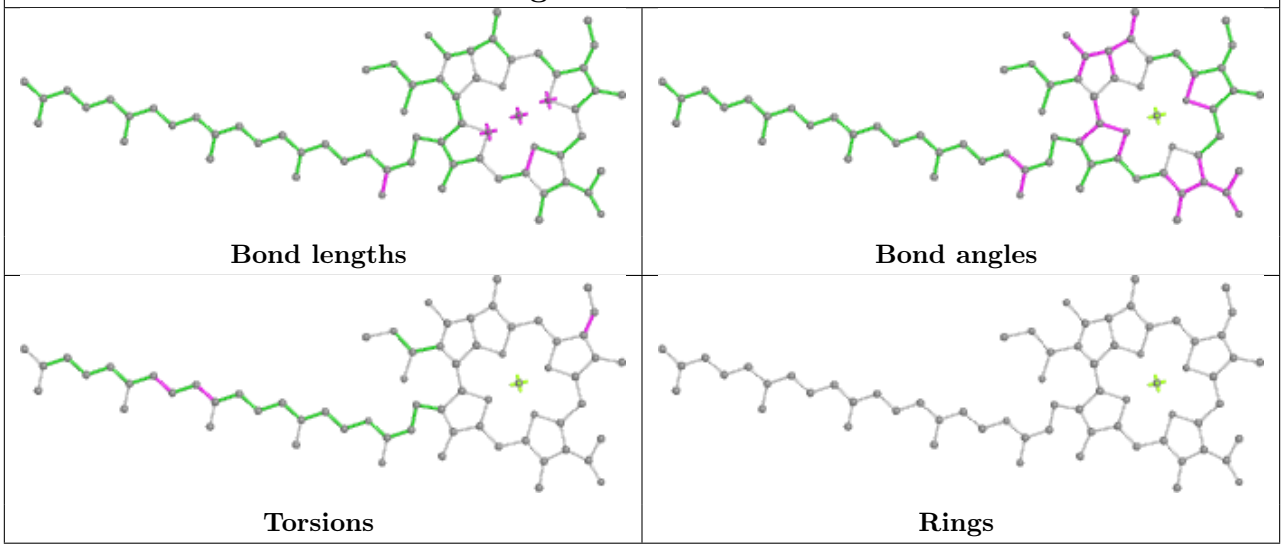


Ligand BPB L 303

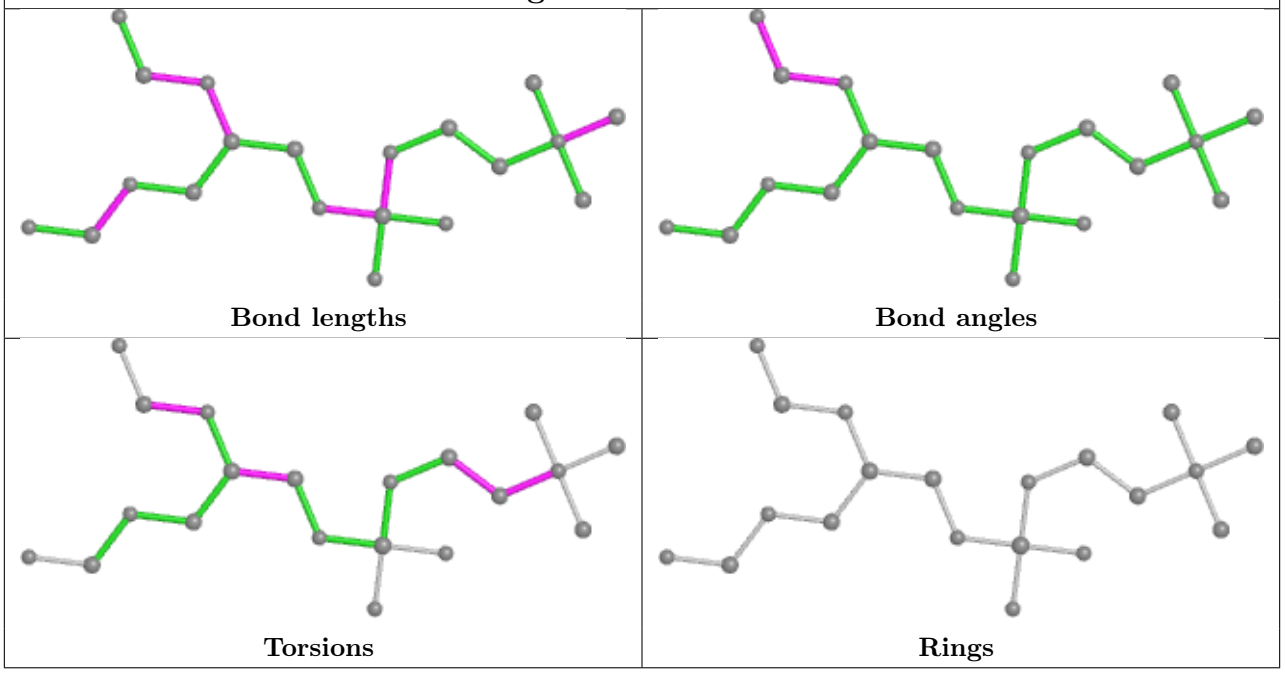
Ligand SPO G 101



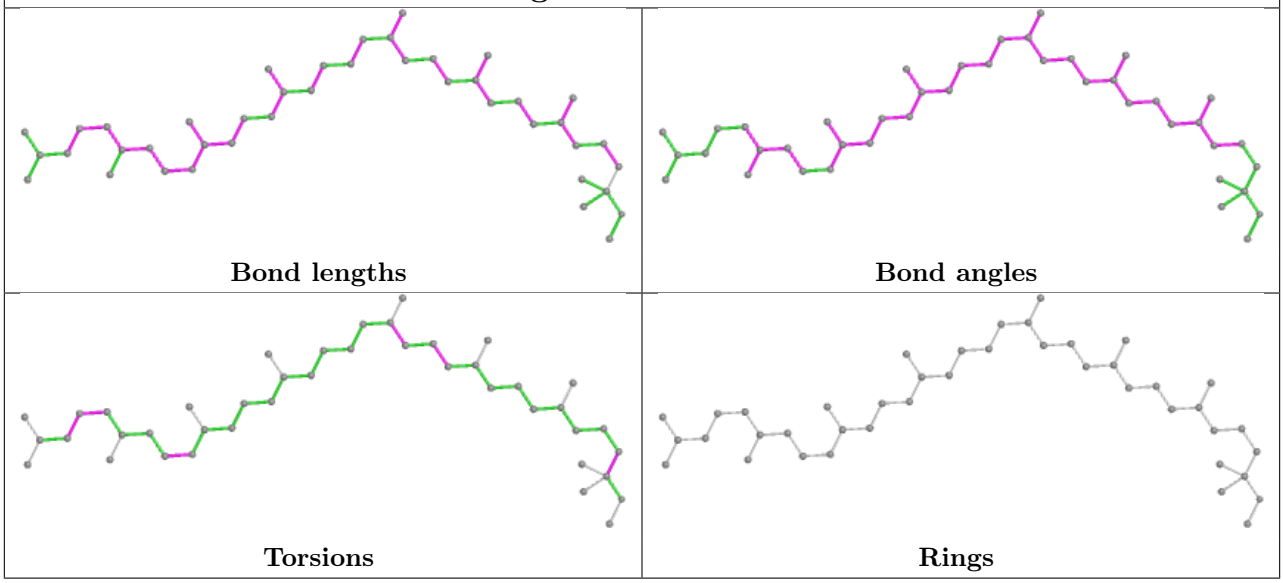
Ligand BCL 9 101



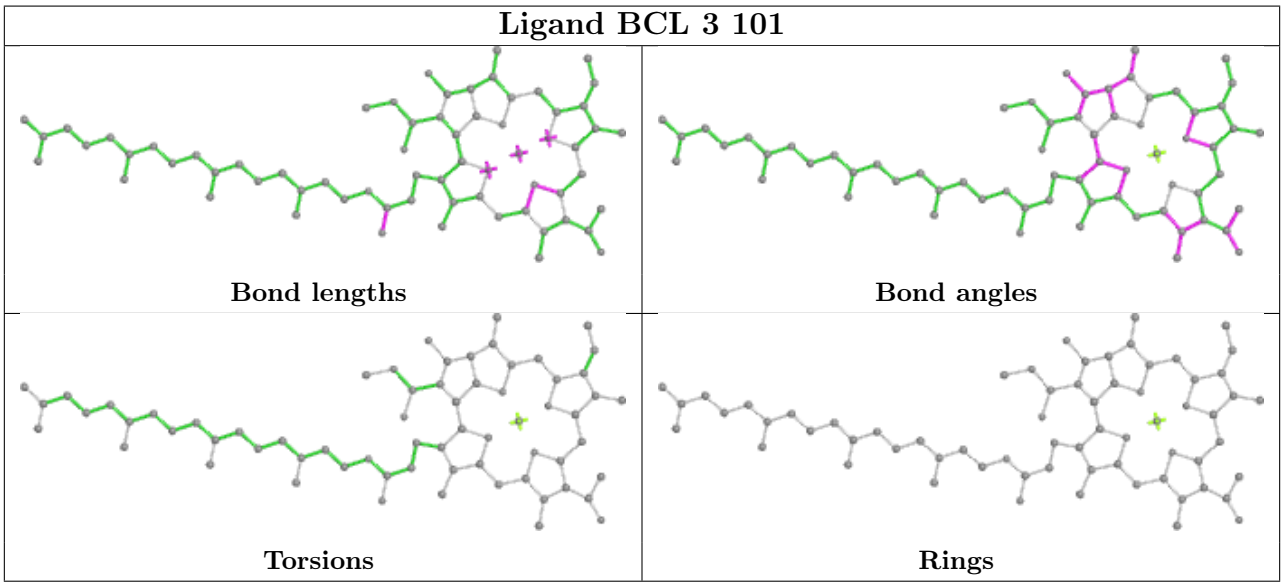
Ligand PC1 H 303



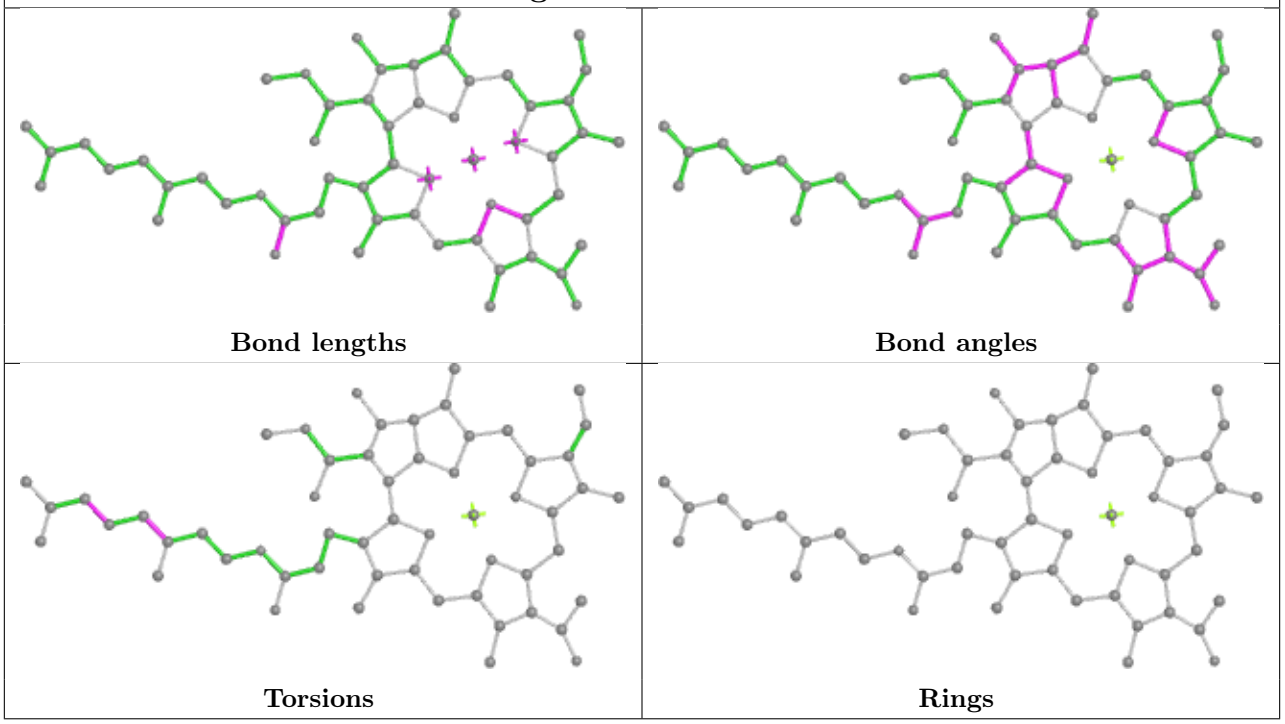
Ligand SPO 3 102



Ligand BCL 3 101

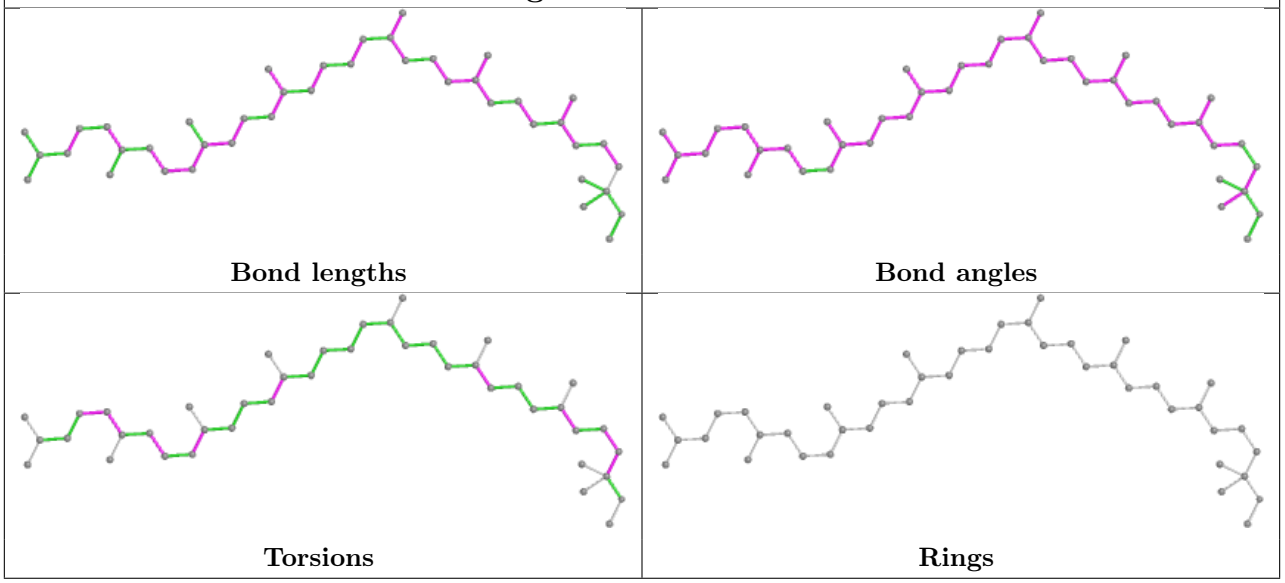


Ligand BCL 1 101

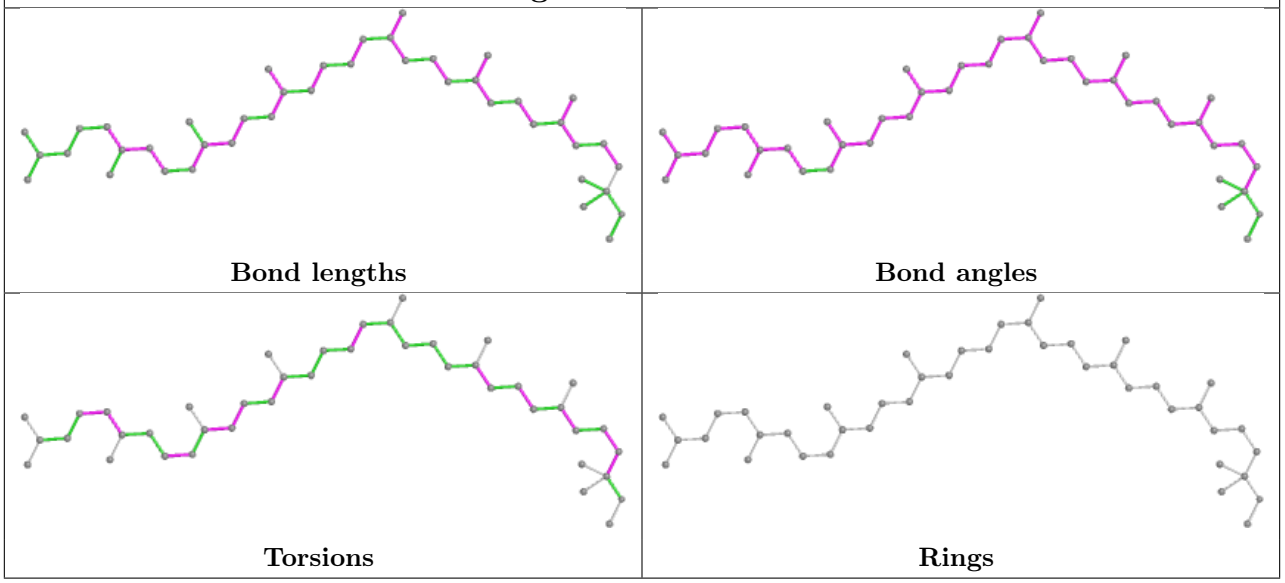


Ligand SPO P 101

Ligand SPO V 101



Ligand SPO J 101



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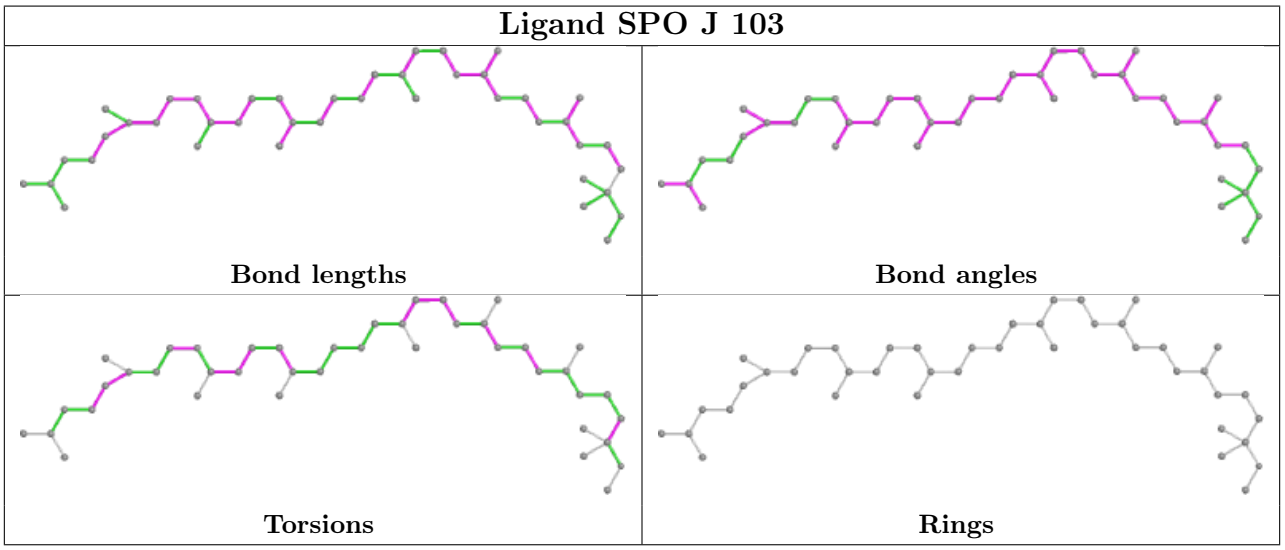
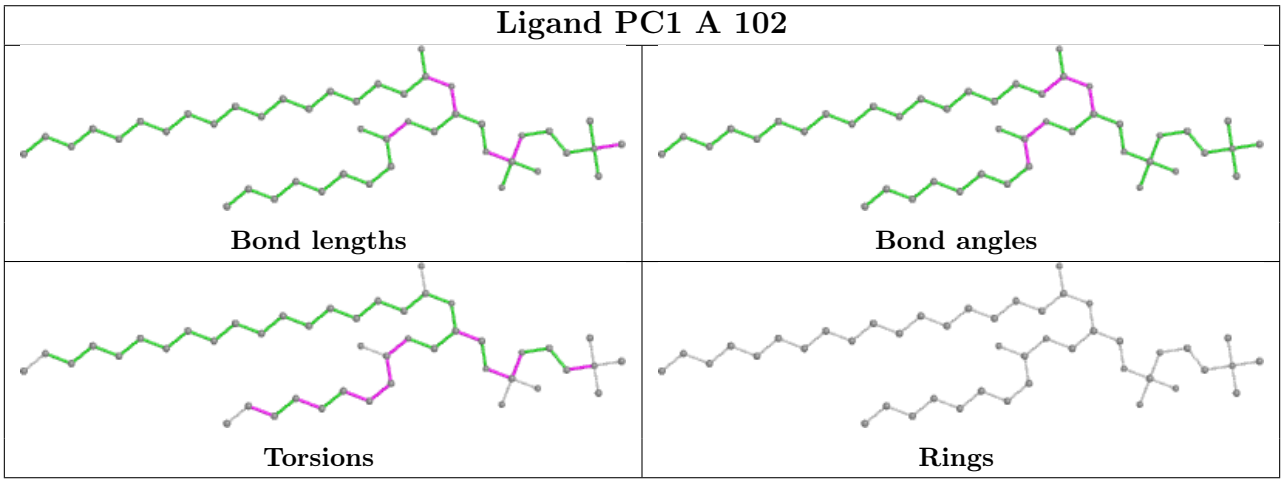
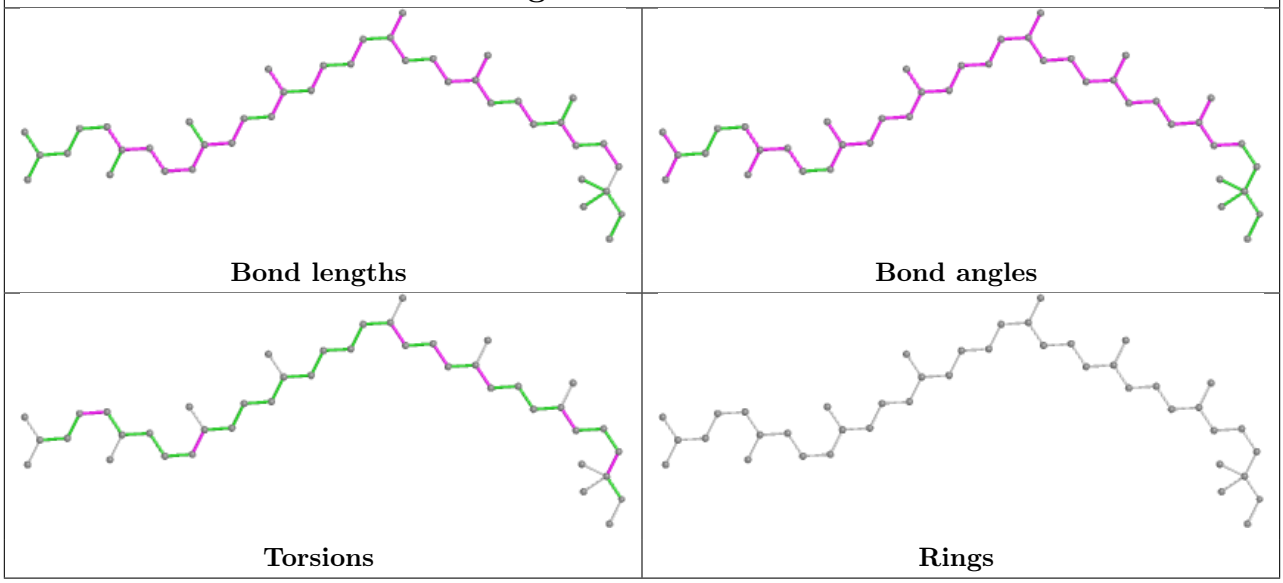


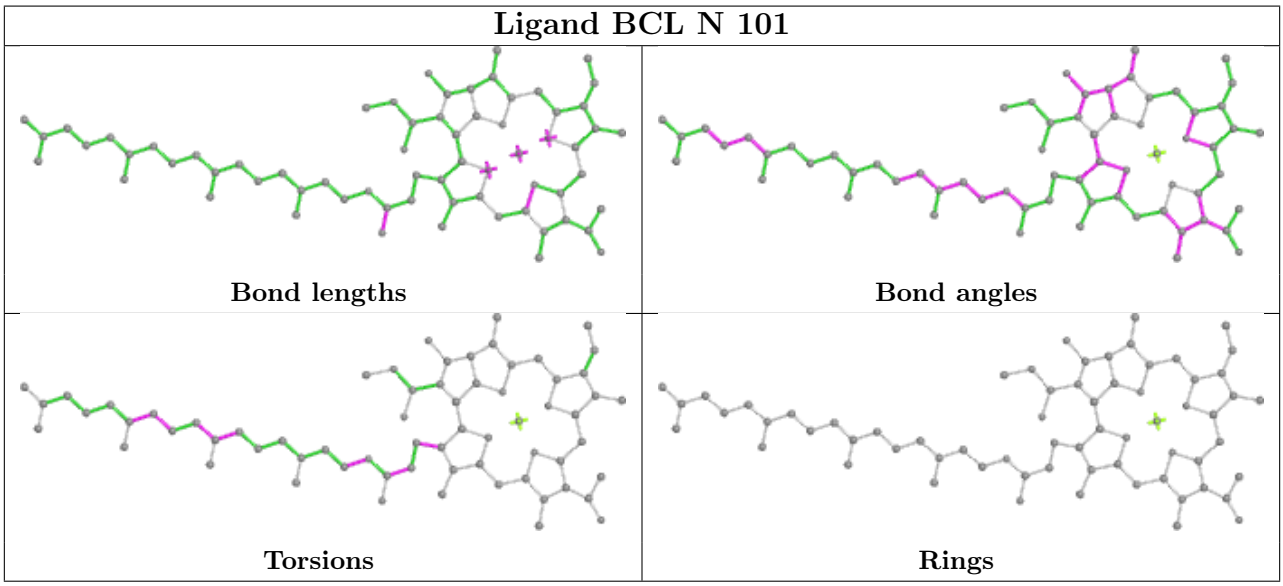
Ligand PC1 A 102



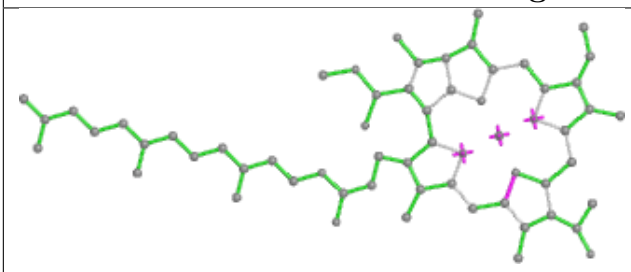
Ligand SPO E 102



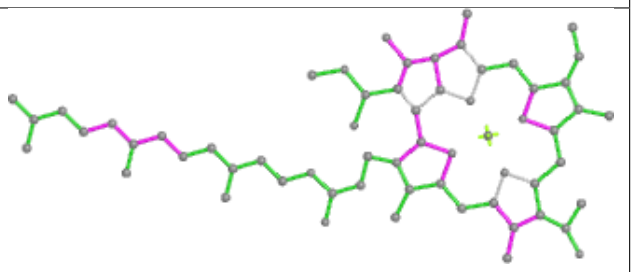
Ligand BCL N 101



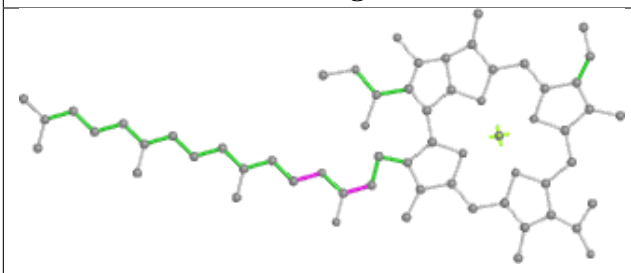
Ligand BCL 8 101



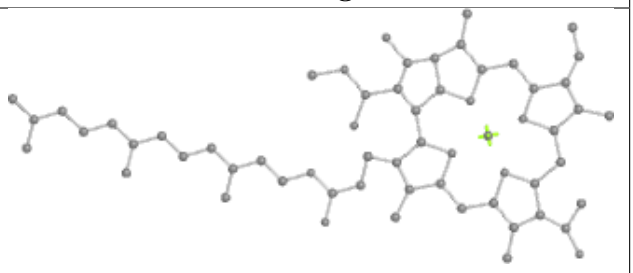
Bond lengths



Bond angles

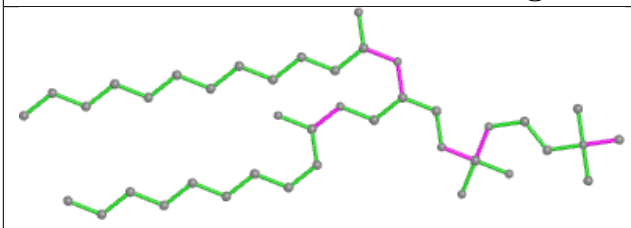


Torsions

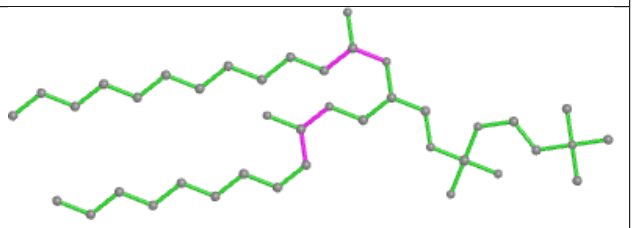


Rings

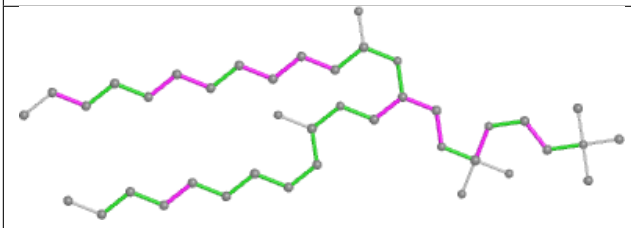
Ligand PC1 H 301



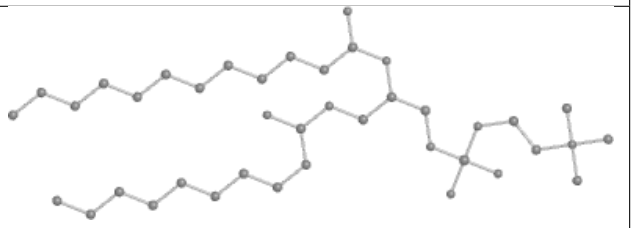
Bond lengths



Bond angles

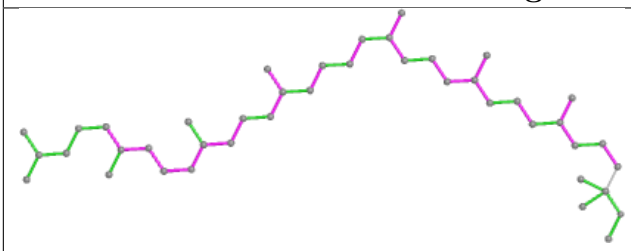


Torsions

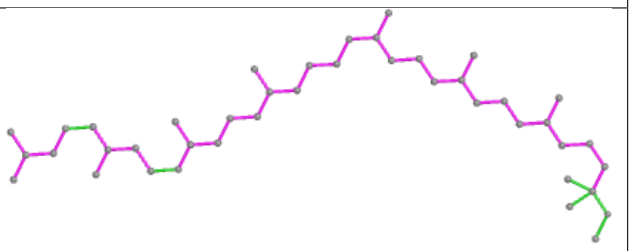


Rings

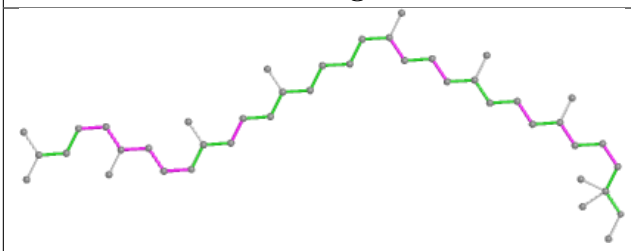
Ligand SPO D 103



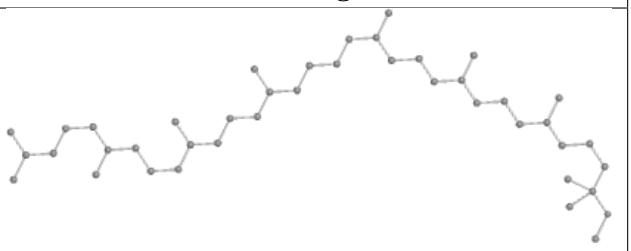
Bond lengths



Bond angles

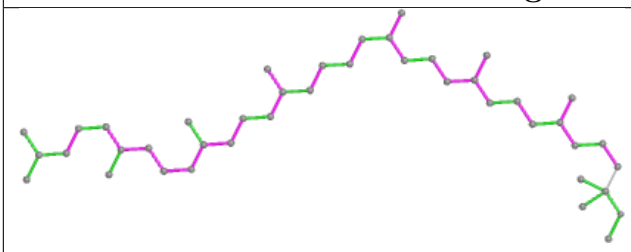


Torsions

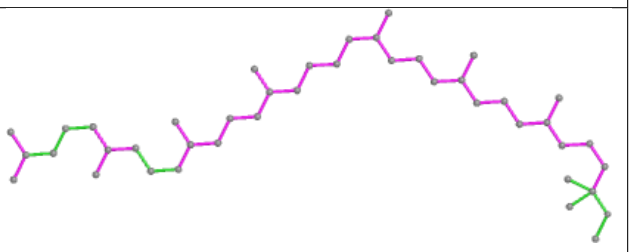


Rings

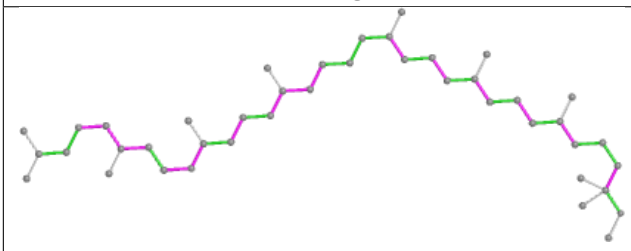
Ligand SPO N 102



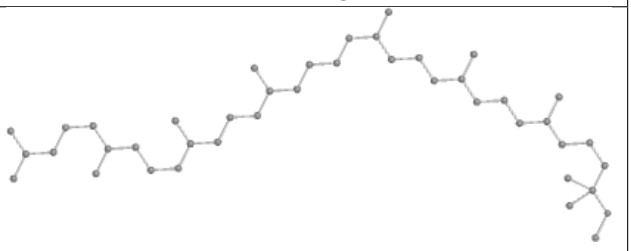
Bond lengths



Bond angles

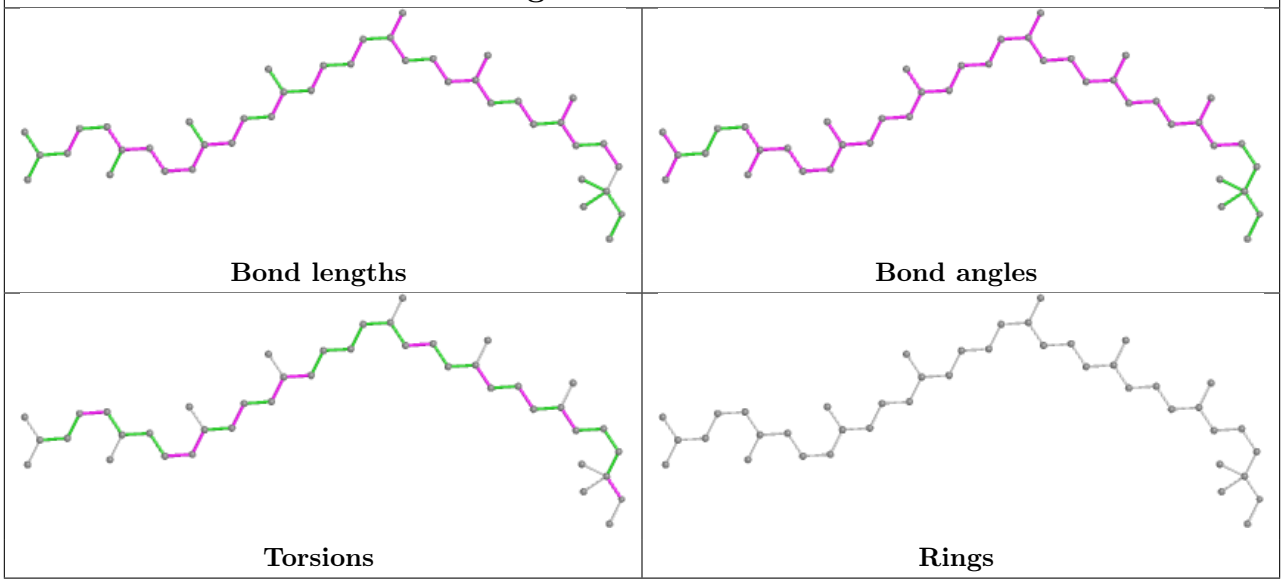


Torsions

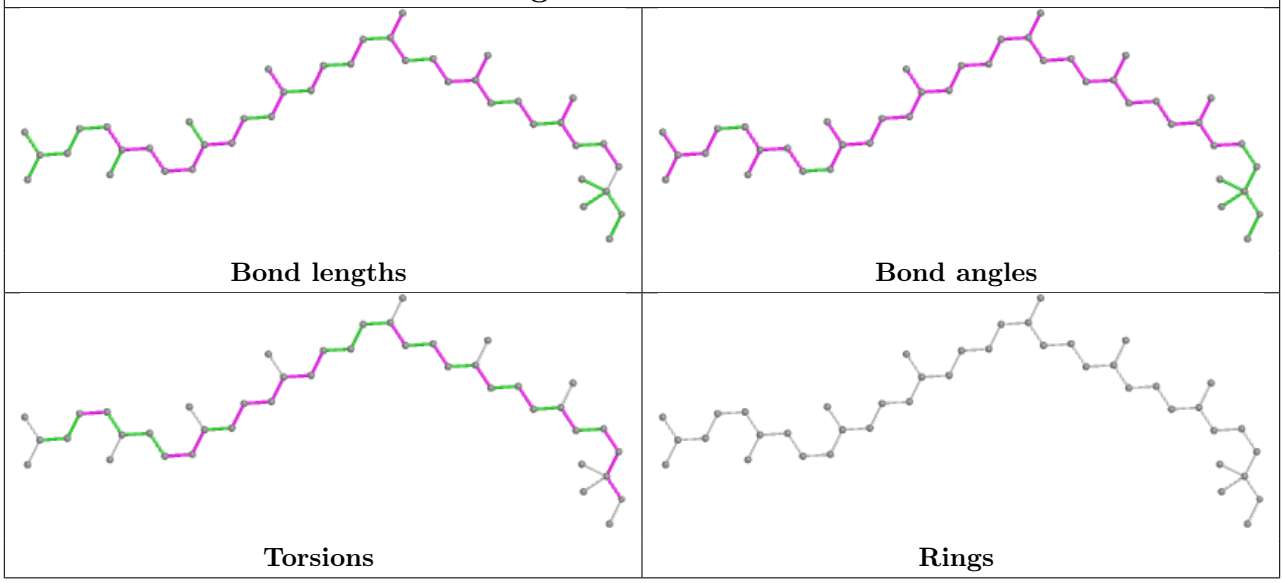


Rings

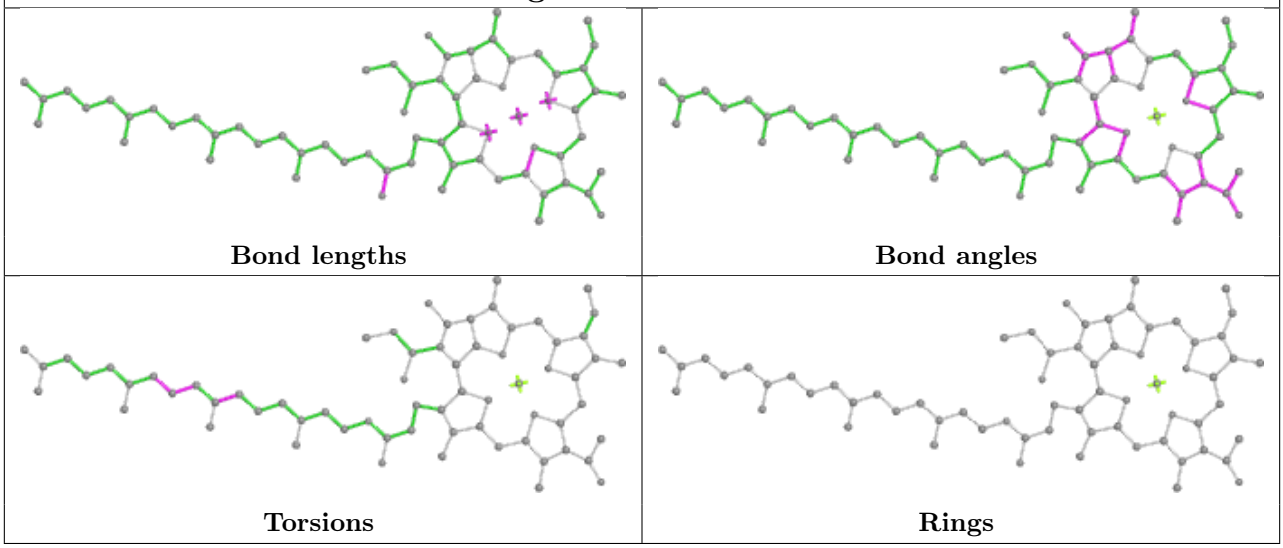
Ligand SPO T 102



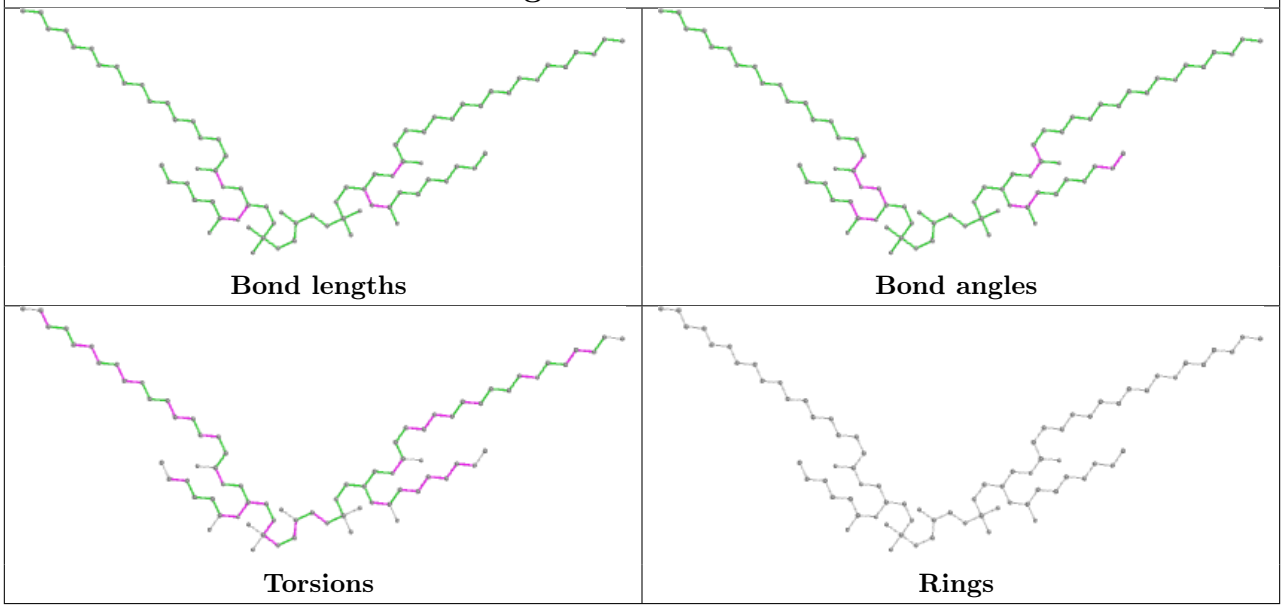
Ligand SPO 8 102



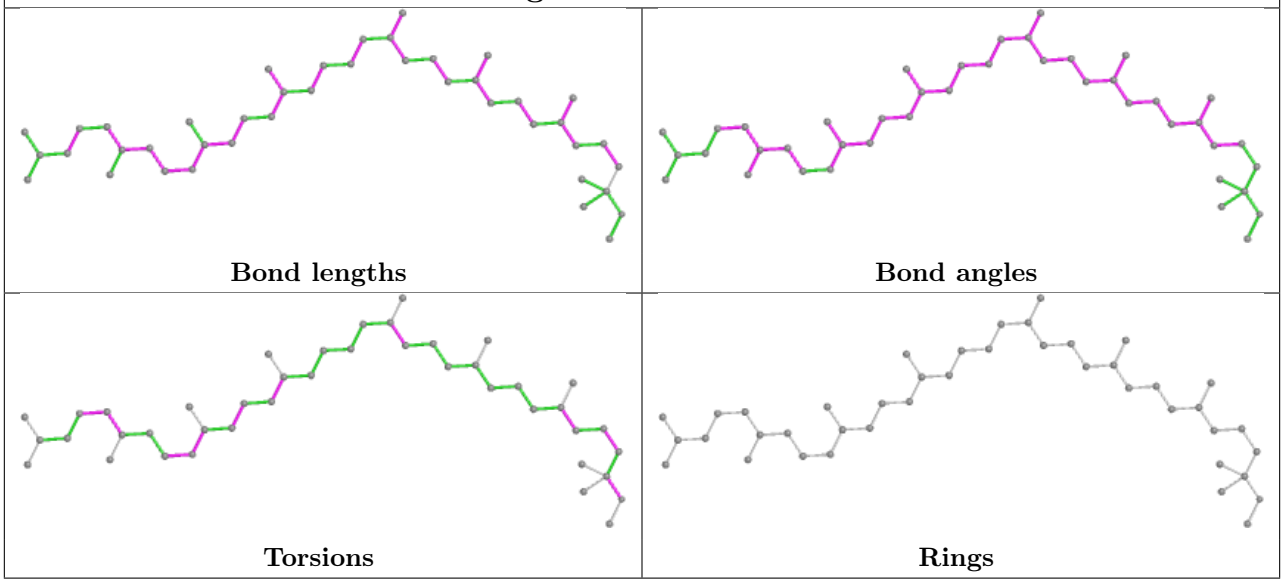
Ligand BCL F 101



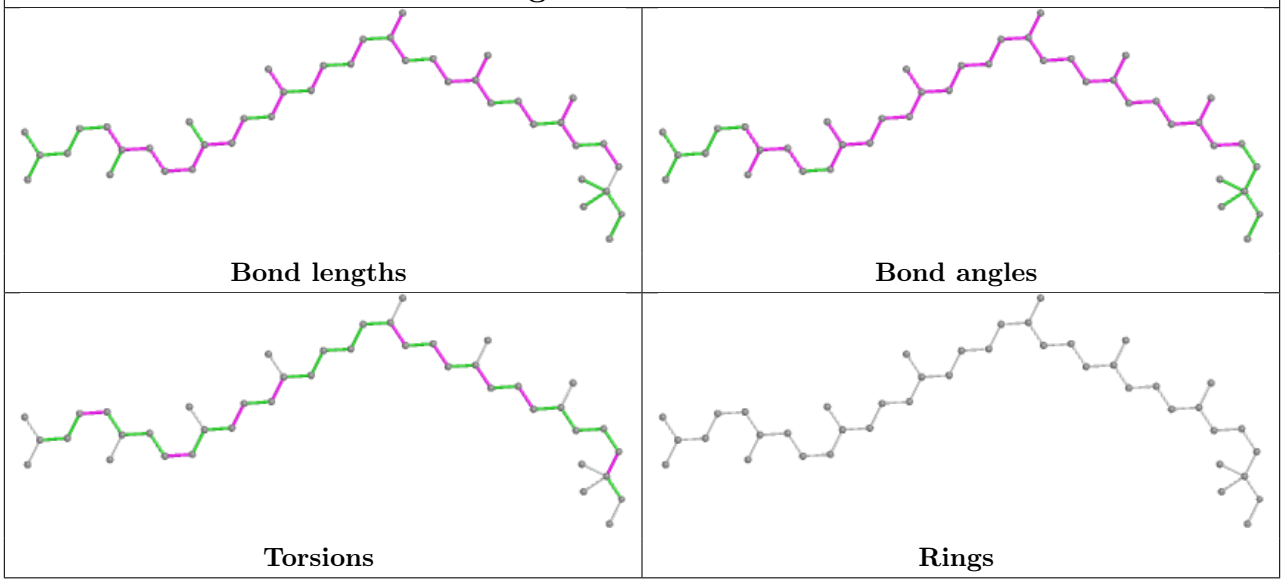
Ligand CDL H 304

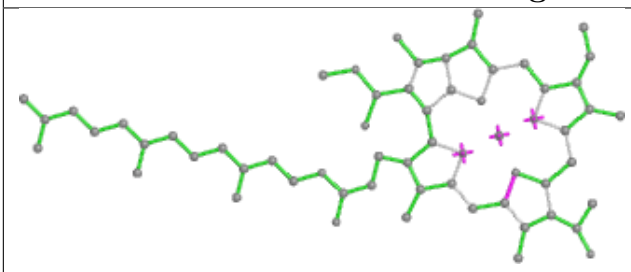
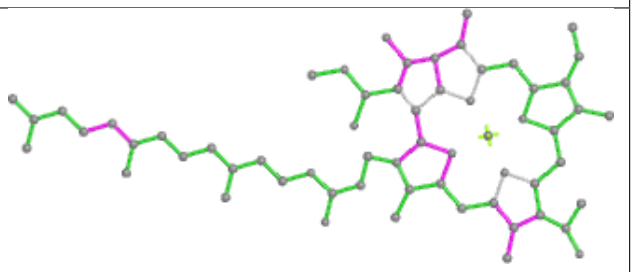
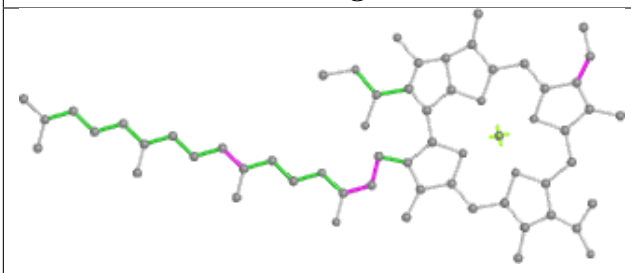
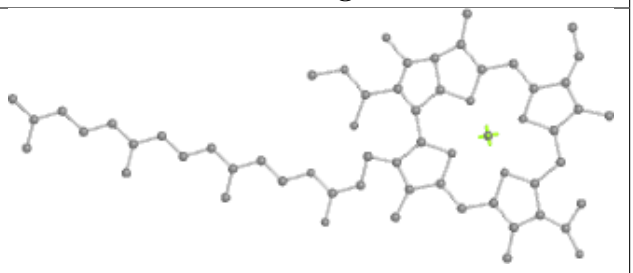


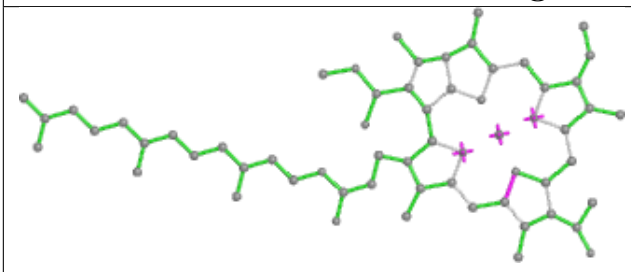
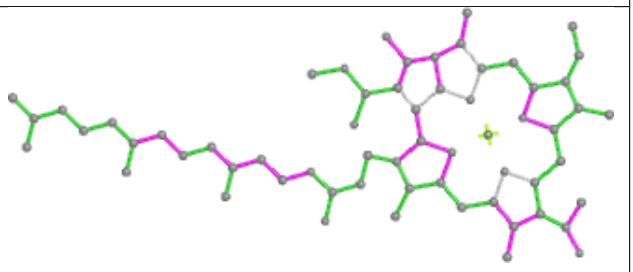
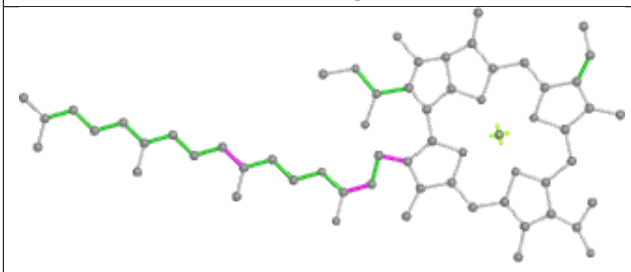
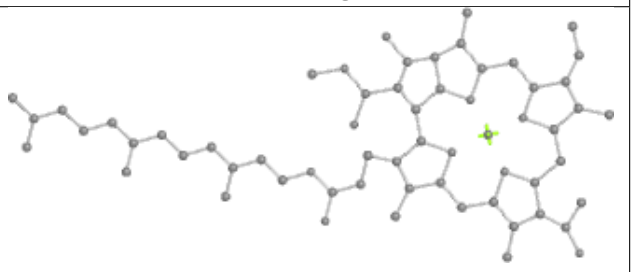
Ligand SPO O 104



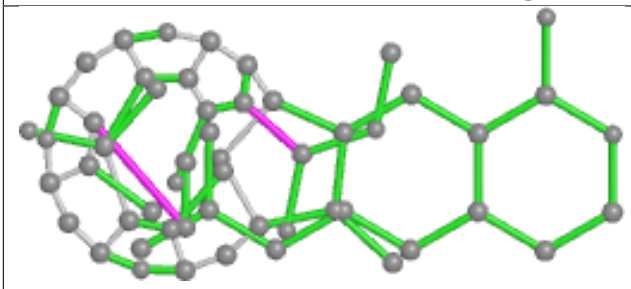
Ligand SPO F 102



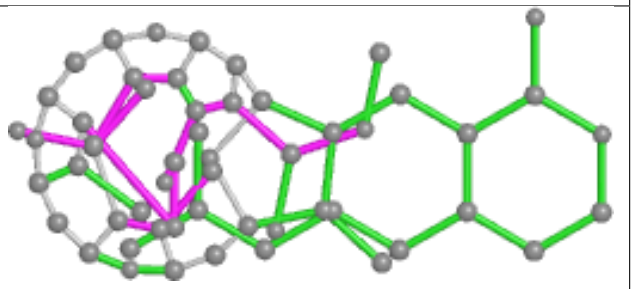
Ligand BCL 1 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 0 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

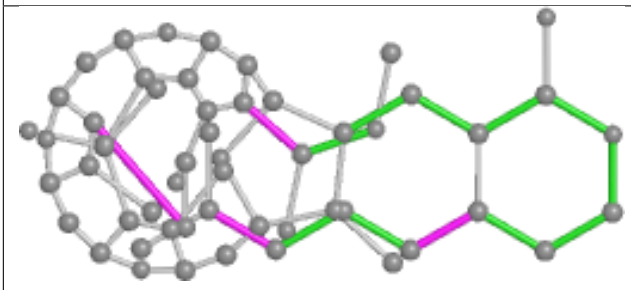
Ligand BPB M 403



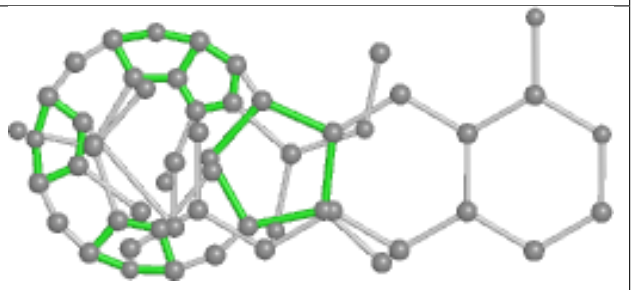
Bond lengths



Bond angles

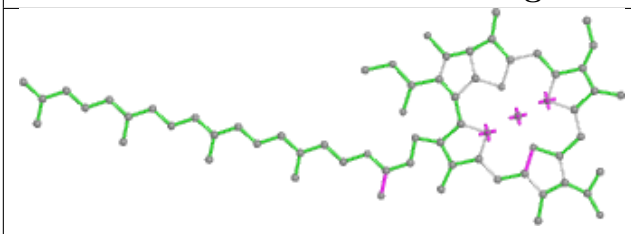


Torsions

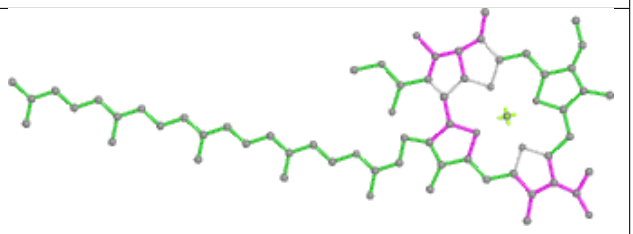


Rings

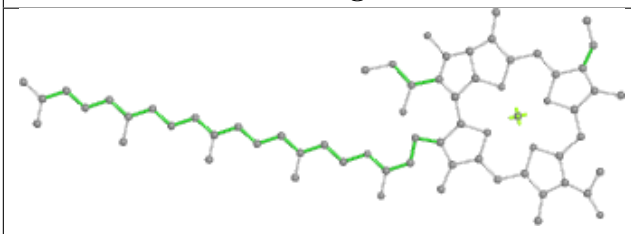
Ligand BCL D 101



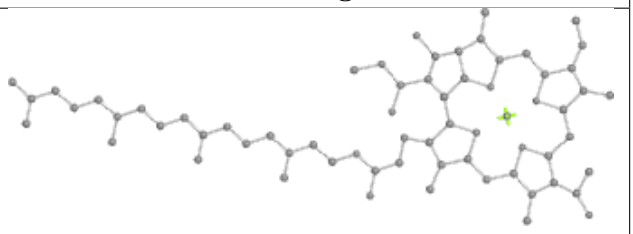
Bond lengths



Bond angles

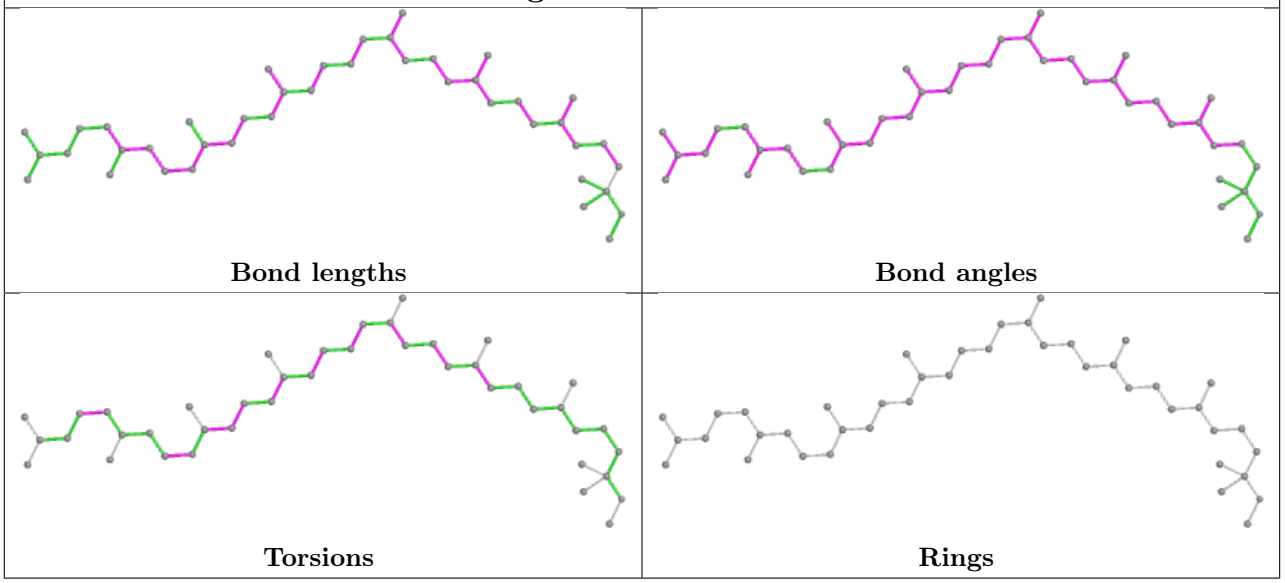


Torsions

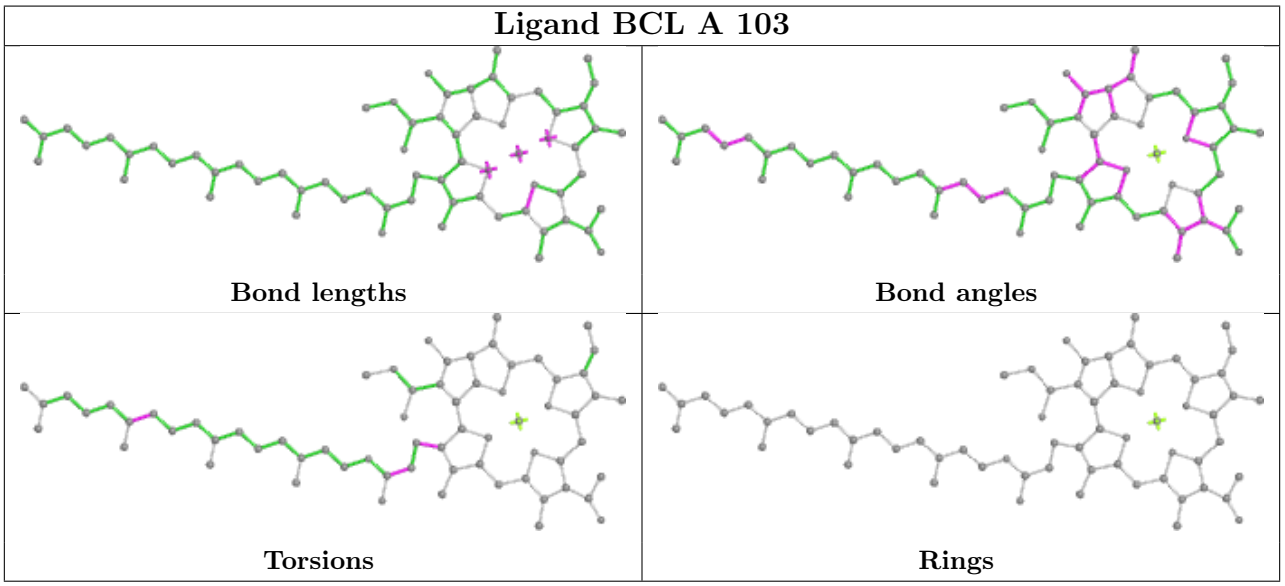


Rings

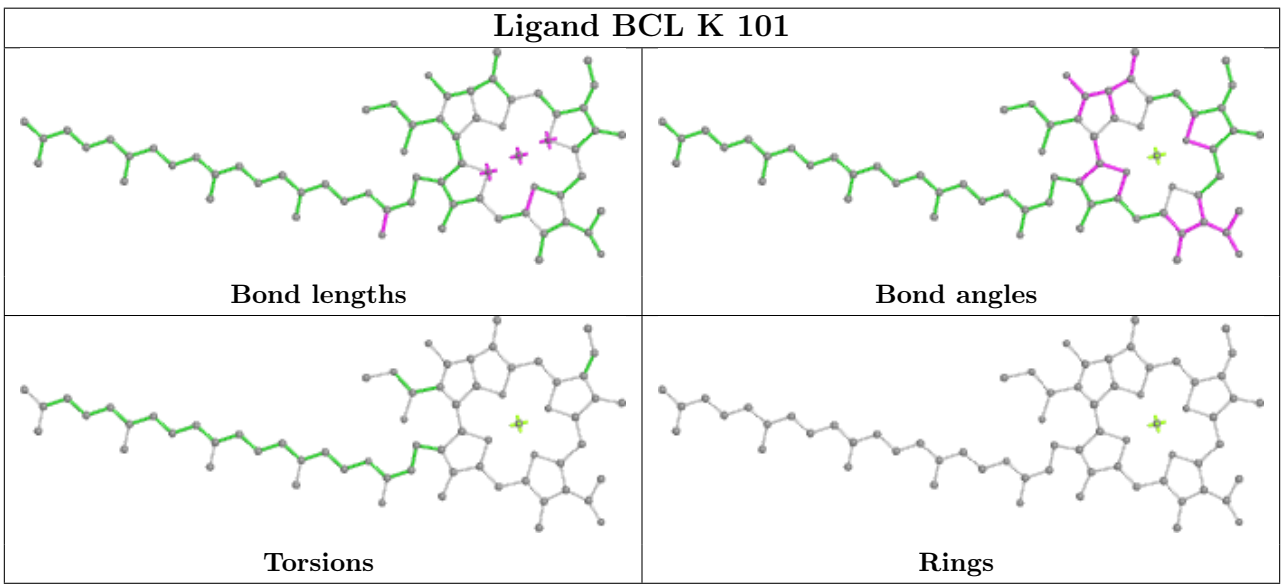
Ligand SPO B 101



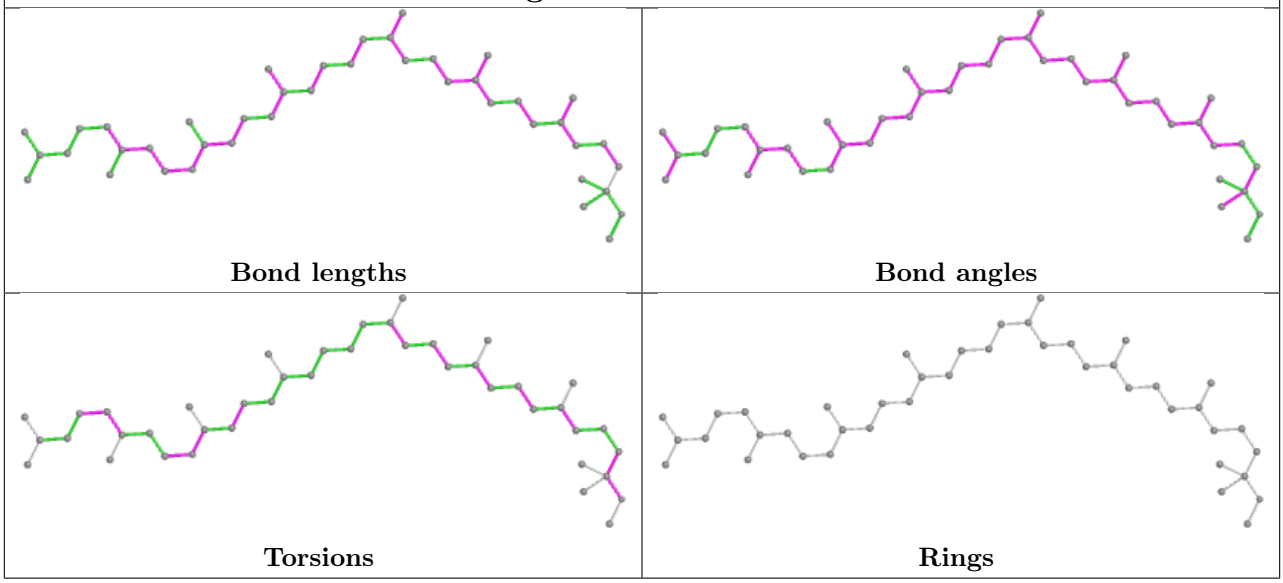
Ligand BCL A 103



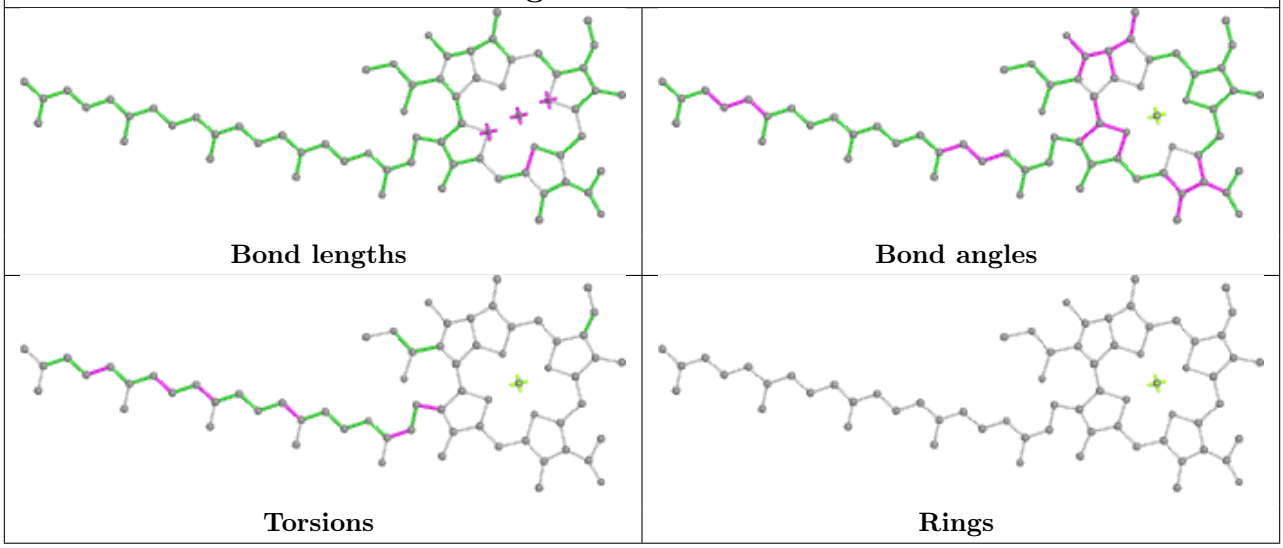
Ligand BCL K 101



Ligand SPO U 104



Ligand BCL C 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

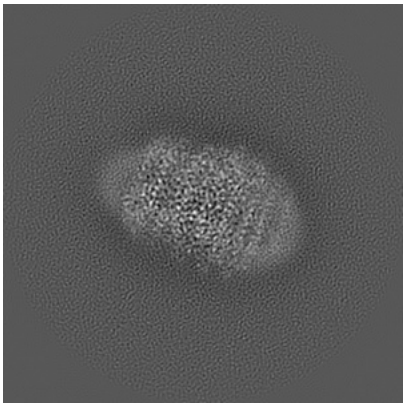
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32047. These allow visual inspection of the internal detail of the map and identification of artifacts.

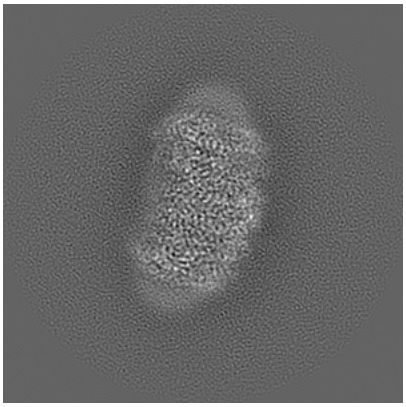
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

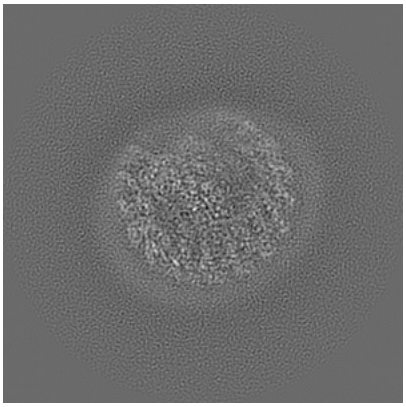
6.1.1 Primary map



X



Y

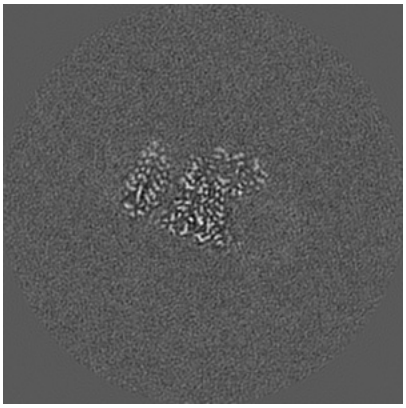


Z

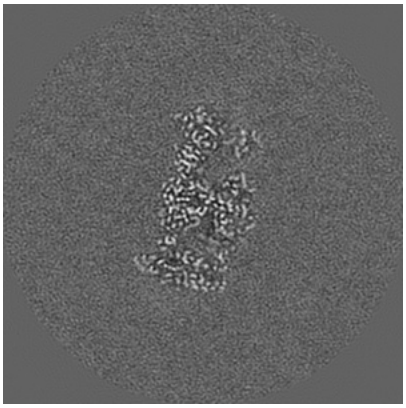
The images above show the map projected in three orthogonal directions.

6.2 Central slices

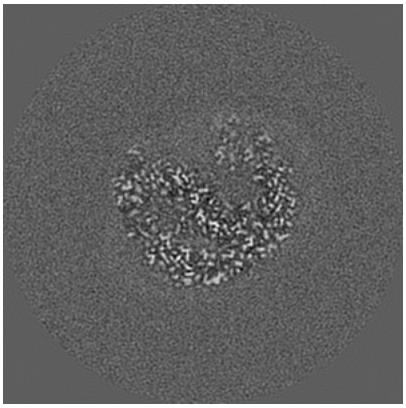
6.2.1 Primary map



X Index: 125



Y Index: 125

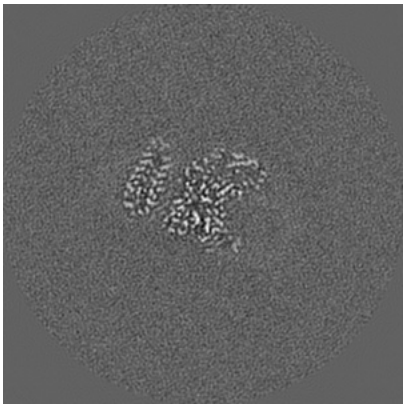


Z Index: 125

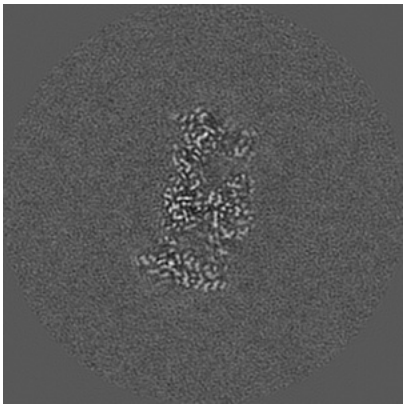
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

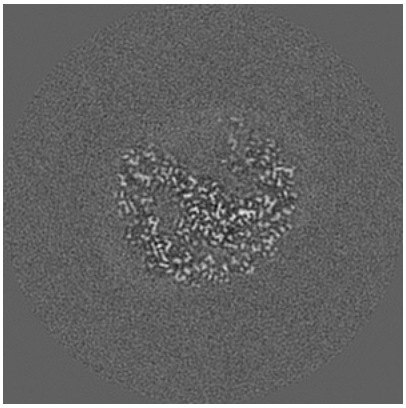
6.3.1 Primary map



X Index: 126



Y Index: 124

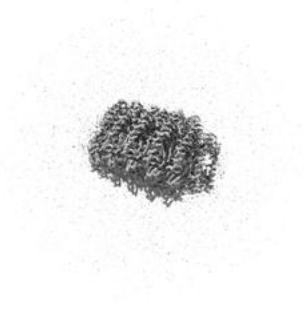


Z Index: 119

The images above show the largest variance slices of the map in three orthogonal directions.

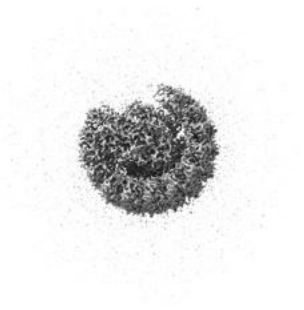
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

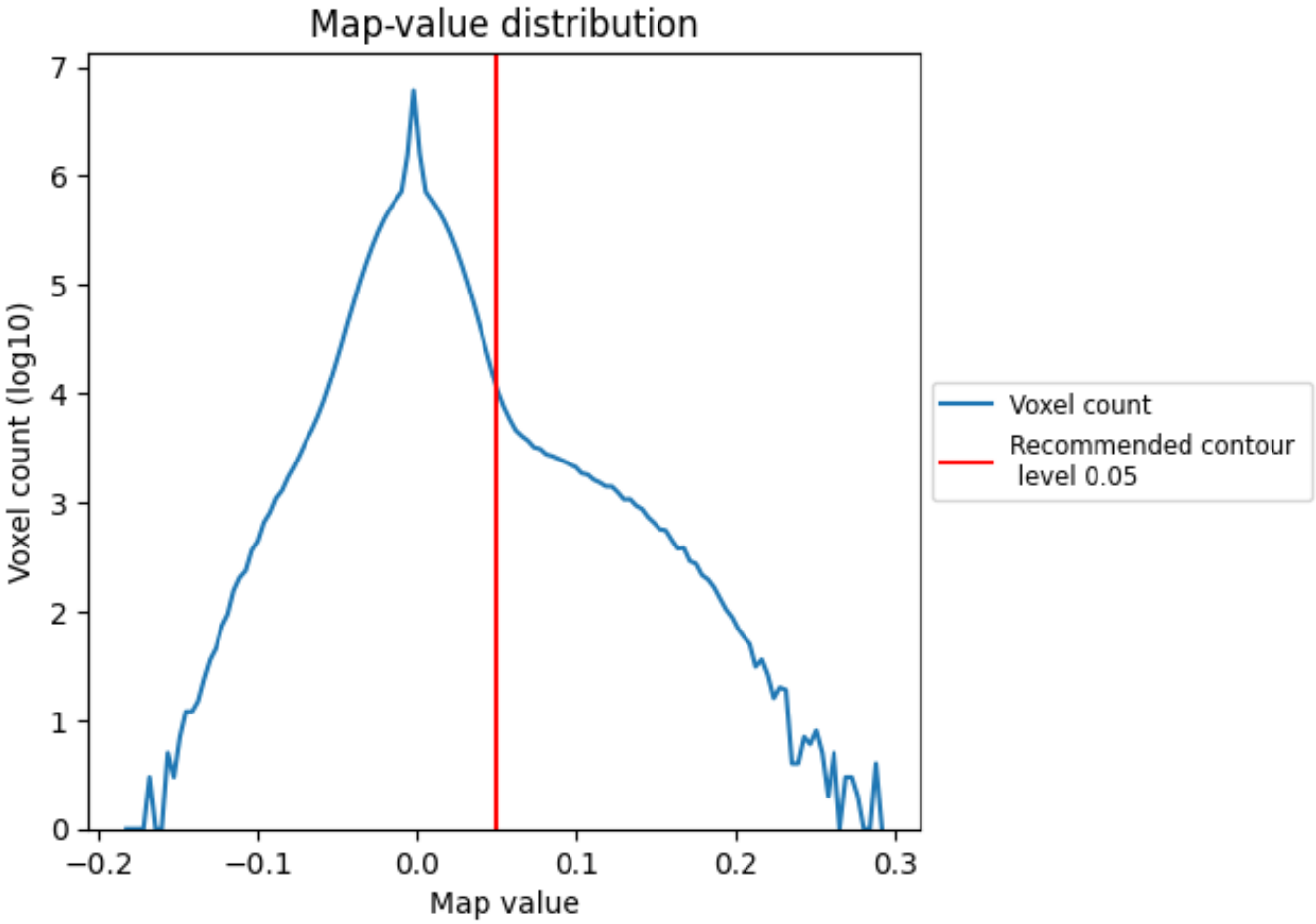
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

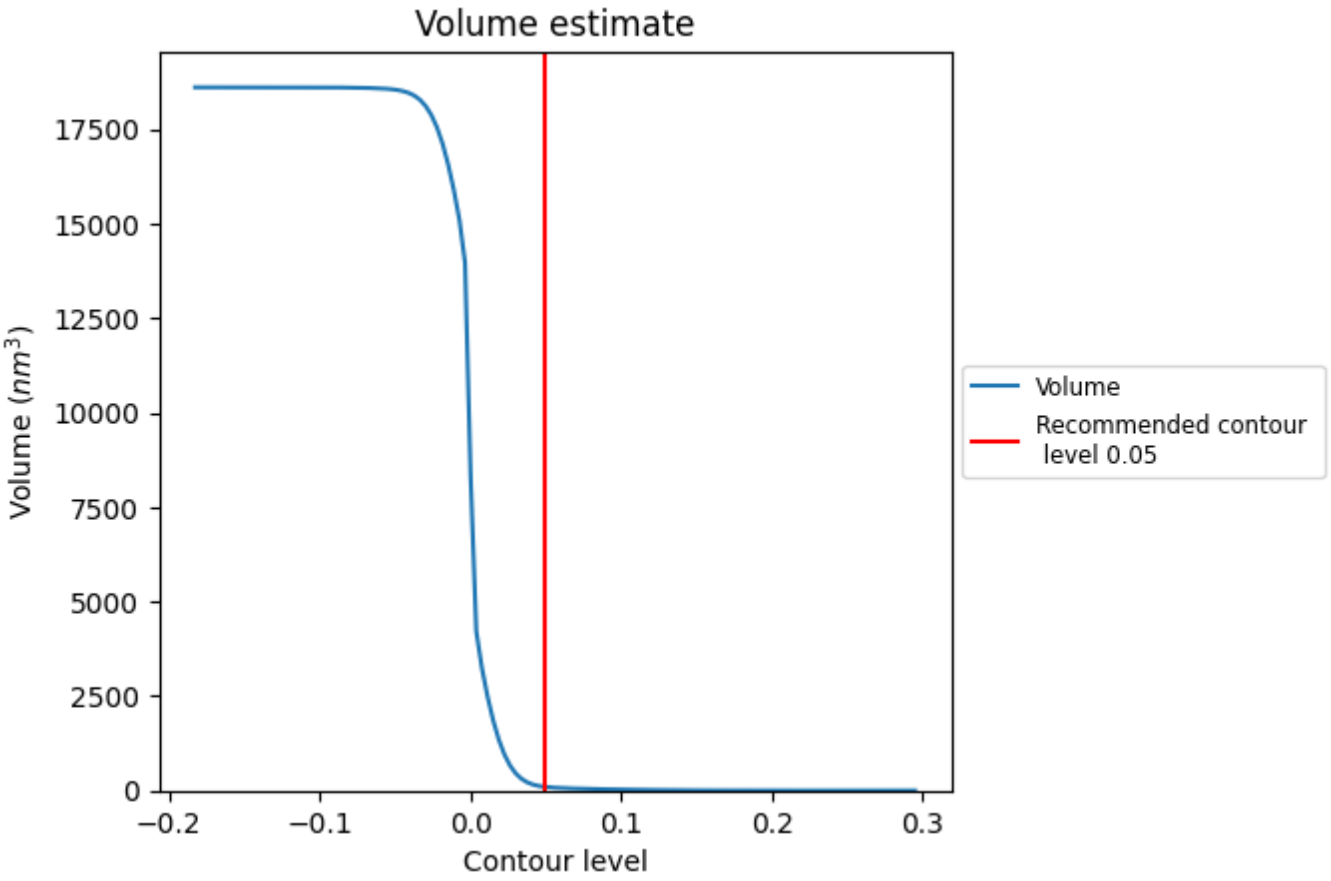
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

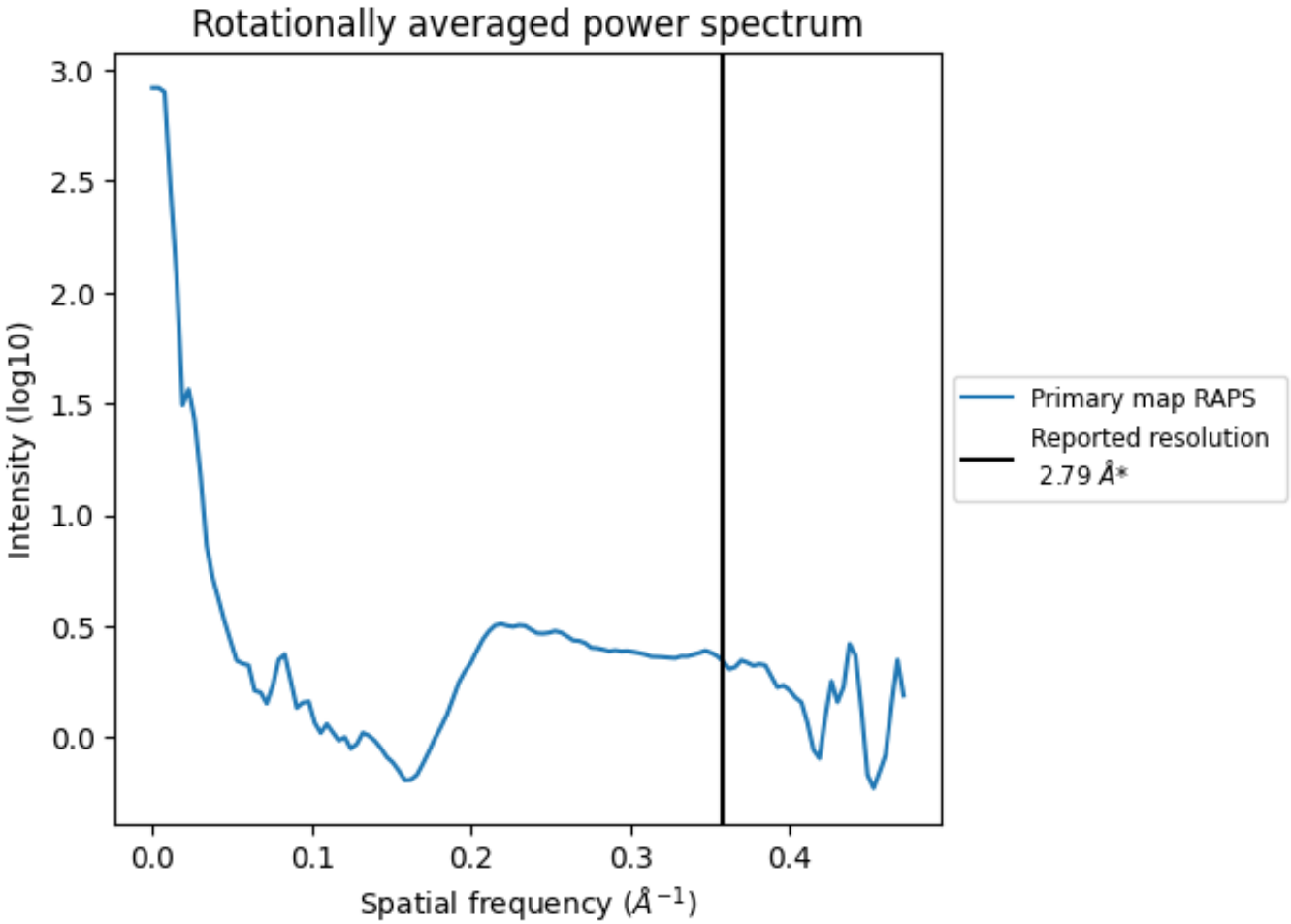
7.2 Volume estimate



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 87 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

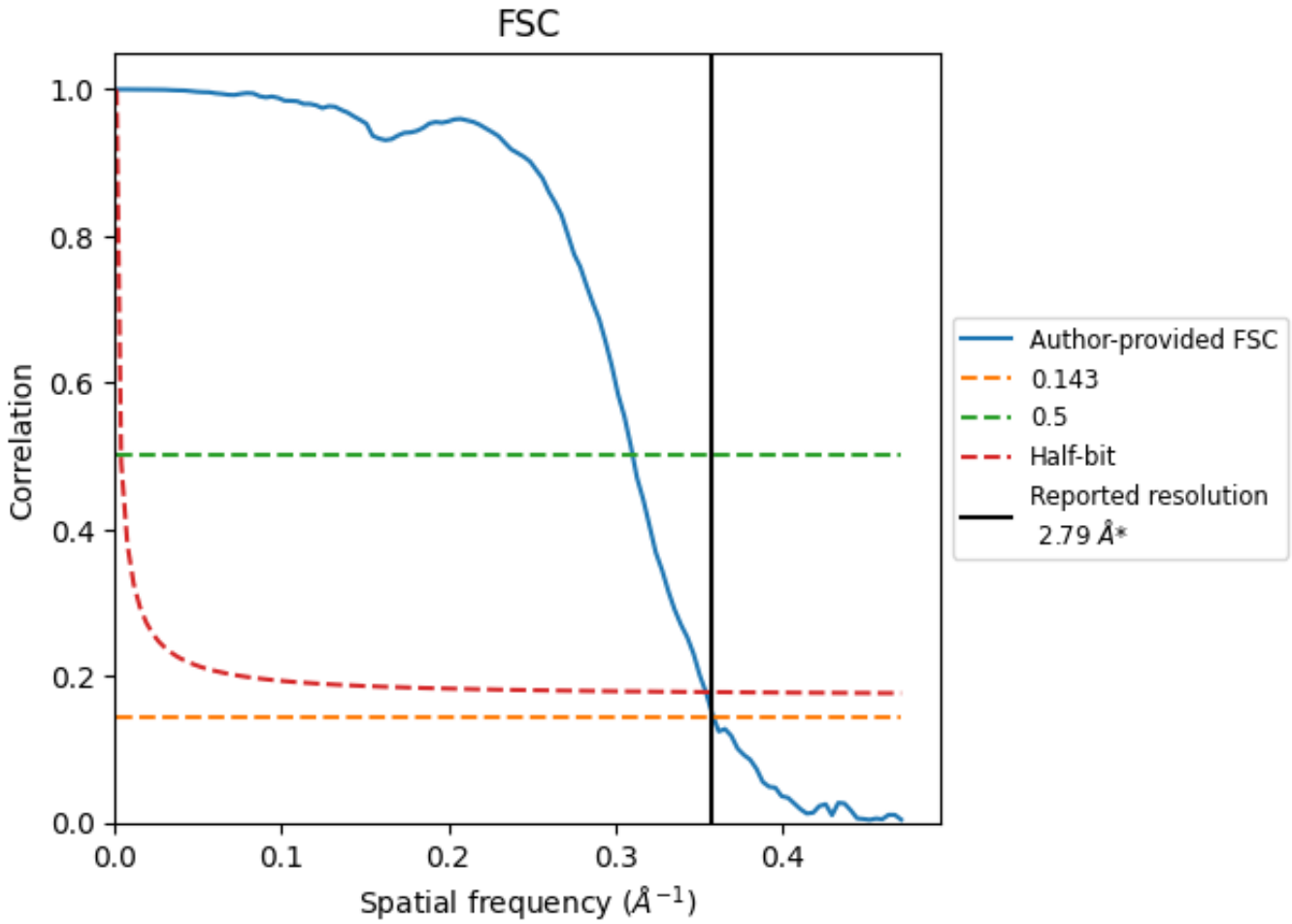


*Reported resolution corresponds to spatial frequency of 0.358 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.358 Å^{-1}

8.2 Resolution estimates (i)

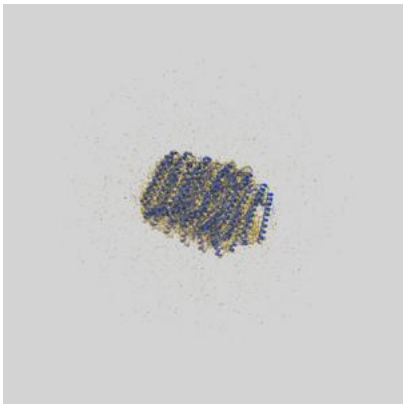
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.78	3.22	2.82
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

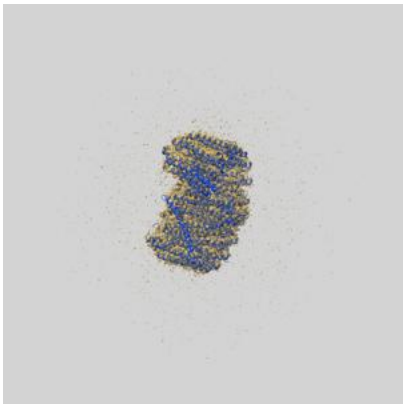
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32047 and PDB model 7VNY. Per-residue inclusion information can be found in section 3 on page 15.

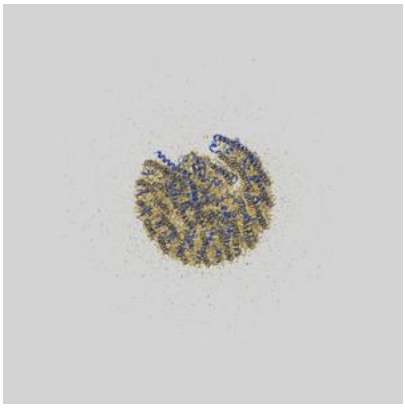
9.1 Map-model overlay



X



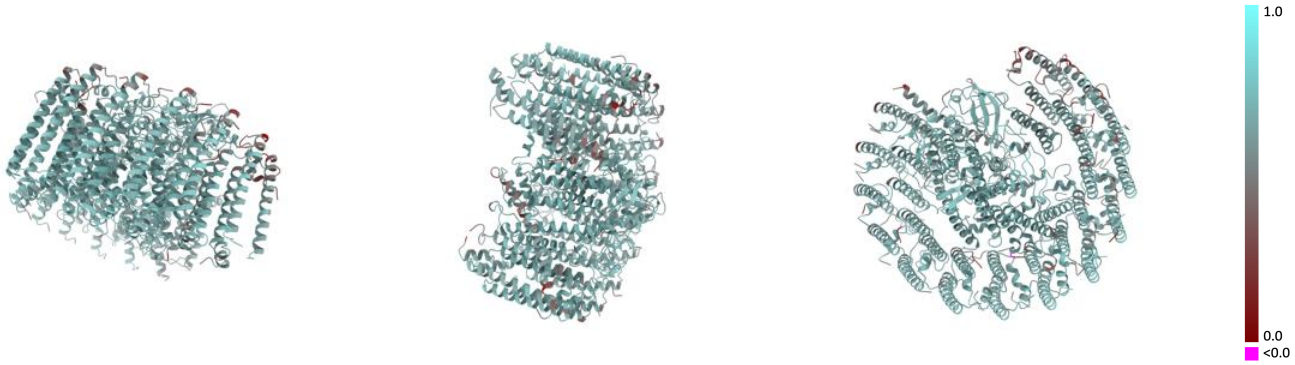
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

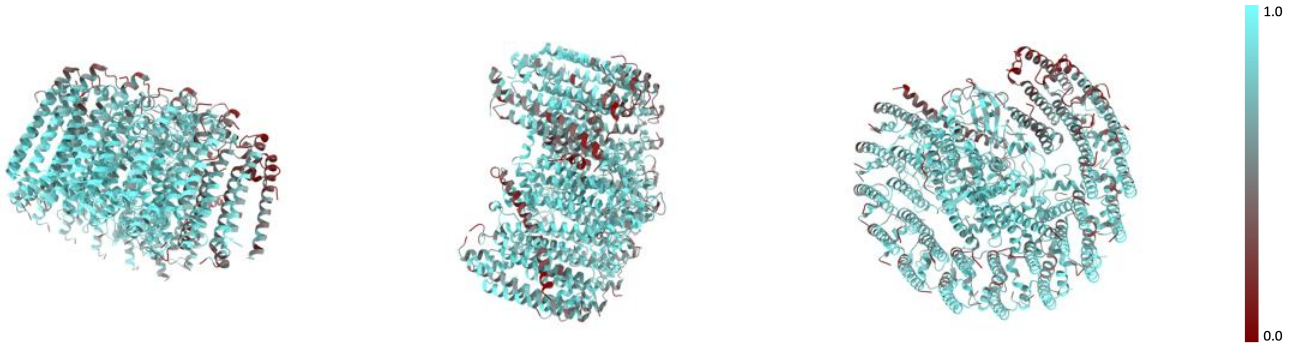
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

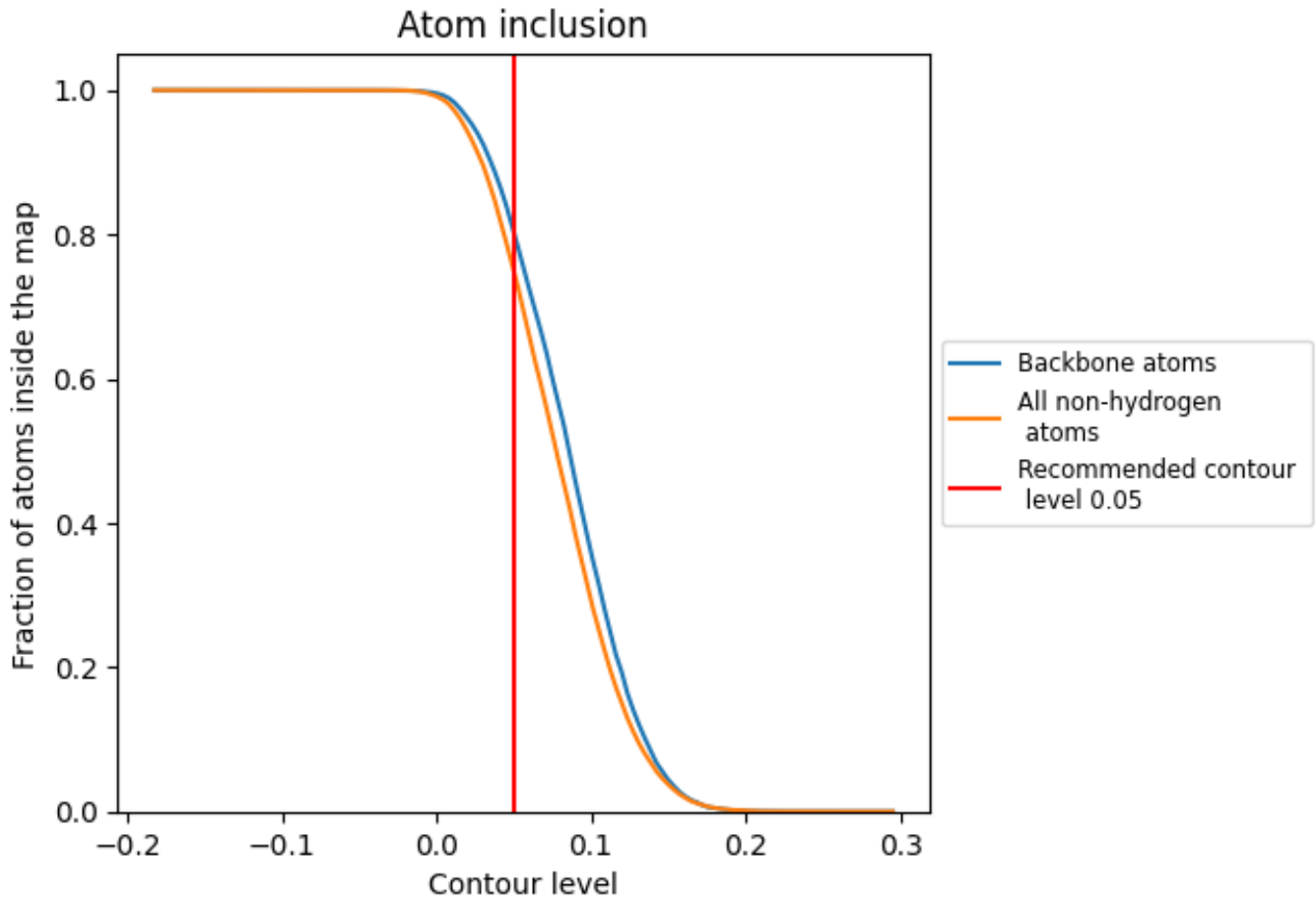
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7491	0.6330
0	0.7711	0.6240
1	0.4771	0.5590
2	0.3948	0.5260
3	0.6426	0.6080
7	0.6973	0.6110
8	0.6133	0.5870
9	0.8011	0.6460
A	0.7780	0.6500
B	0.7820	0.6390
C	0.6568	0.5890
D	0.7624	0.6440
E	0.7405	0.6150
F	0.8098	0.6530
G	0.7325	0.6280
H	0.7058	0.6330
I	0.8102	0.6510
J	0.7342	0.6160
K	0.7945	0.6440
L	0.8698	0.6720
M	0.8937	0.6800
N	0.7069	0.6110
O	0.7868	0.6380
P	0.6935	0.6020
Q	0.7866	0.6380
R	0.7383	0.6240
S	0.8187	0.6460
T	0.7002	0.6100
U	0.7975	0.6340
V	0.7013	0.6010
W	0.6991	0.6220
X	0.3364	0.5130
Y	0.5533	0.5940
Z	0.5731	0.5580